

chain nodes :

12 13 14 15 27 28 29 30 31 32

ring nodes :

1 2 3 4 5 6 7 8 9 10 11

ring/chain nodes :

26

chain bonds :

2-26 5-31 7-29 10-27 12-13 14-15 27-28 29-30 31-32

ring bonds :

1-2 1-11 2-3 3-4 4-5 5-6 6-7 7-8 8-9 9-10 10-11

exact/norm bonds :

1-2 1-11 2-3 2-26 3-4 4-5 5-6 5-31 6-7 7-8 7-29 8-9 9-10  
10-11 10-27 12-13 14-15 27-28 29-30 31-32

G1:[\*1-\*2],[\*3-\*4]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom  
10:Atom 11:Atom 12:CLASS 13:CLASS 14:CLASS 15:CLASS 26:CLASS  
27:CLASS 28:Atom 29:CLASS 30:Atom 31:CLASS 32:Atom

09/762,522

=> d his

(FILE 'HOME' ENTERED AT 10:40:08 ON 09 APR 2002)

FILE 'REGISTRY' ENTERED AT 10:40:14 ON 09 APR 2002

L1               STRUCTURE UPLOADED  
L2               QUE L1  
L3               8 S L2  
L4               SCREEN 1841  
L5               STRUCTURE UPLOADED  
L6               QUE L5 AND L4  
L7               13 S L6  
L8               0 S SZ>7  
L9               4161 S 13/SZ  
L10              14066 S 14/SZ  
L11              7638 S 15/SZ  
L12              10223 S 16/SZ  
L13              1739 S 17/SZ  
L14              8741 S 18/SZ  
L15              13916 S 12/SZ  
L16              60324 S L9 OR L10 OR L11 OR L12 OR L13 OR L14 OR L15  
L17              50 S L6   SUB=L16 SAM  
L18              STRUCTURE UPLOADED  
L19              QUE L18  
L20              7 S L19   SUB=L16 SAM  
L21              84 S L19   SUB=L16 FUL

FILE 'CAPLUS' ENTERED AT 10:50:22 ON 09 APR 2002

L22              3 S L21

FILE 'CAOLD' ENTERED AT 10:50:29 ON 09 APR 2002

L23              0 S L21

FILE 'MARPAT' ENTERED AT 10:50:36 ON 09 APR 2002

FILE 'CAPLUS' ENTERED AT 10:50:58 ON 09 APR 2002

=> d bib abs hitstr l22 1-3

09/762,522

L22 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2002 ACS

AN 2001:300741 CAPLUS

DN 134:296103

TI Preparation of basic monocyclic compounds having NK2 antagonist action

IN Perrotta, Enzo; Giannotti, Danilo; Altamura, Maria; Giuliani, Sandro; Maggi, Carlo Alberto

PA Menarini Ricerche S.P.A., Italy

SO PCT Int. Appl., 24 pp.

CODEN: PIXXD2

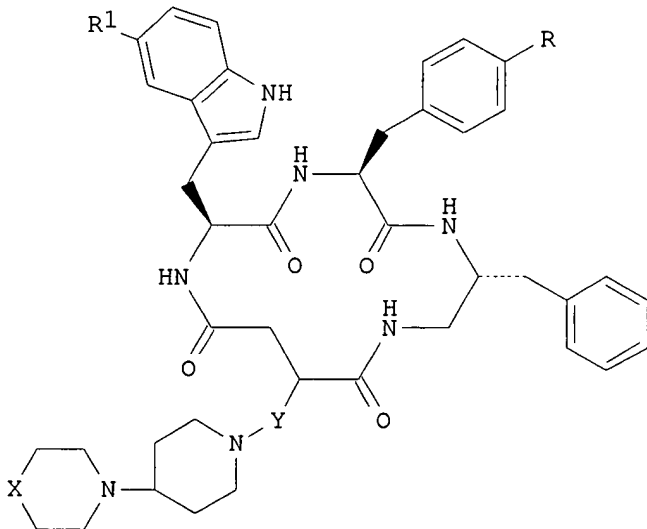
DT Patent

LA English

FAN.CNT 1

no  
US 29  
4-29-02

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2001029066	A2	20010426	WO 2000-EP10181	20001017
	WO 2001029066	A3	20011101		
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	IT 1307809	B1	20011119	IT 1999-FI217	19991021
PRAI	IT 1999-FI217	A	19991021		
OS	MARPAT 134:296103				
GI					



AB Basic monocyclic compds. I [X = CH<sub>2</sub>, O, S, or S(O); Y = CH<sub>2</sub>CONH or CO; R, R<sub>1</sub> = H or halo] and their pharmaceutically acceptable salts, including the resp. diastereoisomers and their mixts., were prepd. as NK-2 antagonists.

Thus, cyclo{-Suc[1-(R)-2(1,4')bipiperidinyl-1'-ylacetyl-amino]-Trp-Phe-[(R)-NH-CH(CH<sub>2</sub>Ph)CH<sub>2</sub>NH]} (I; R = R<sub>1</sub> = H, Y = CH<sub>2</sub>CONH, X = CH<sub>2</sub>; C-Y has R the configuration) was prepd. by coupling of cyclo{-Suc[1-(R)-amino]-Trp-Phe-[(R)-NHCH(CH<sub>2</sub>Ph)CH<sub>2</sub>NH]} with 4-(piperidinyl)piperidine-1-acetic acid hydrochloride (syntheses given). The product was assayed as antagonist to the NK-2 receptor of tachykinins (binding const. pK<sub>i</sub> = 9.4).

IT 334941-96-7P 334941-97-8P 334941-98-9P

334941-99-0P 334942-00-6P 334942-01-7P

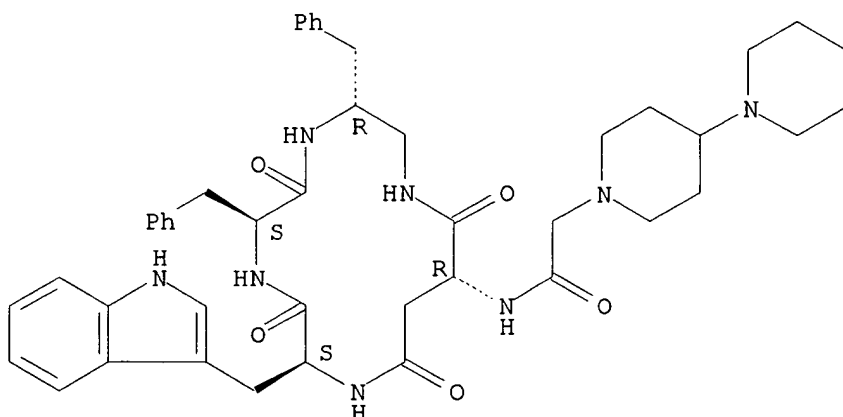
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of basic monocyclic compds. having NK2 antagonist action)

RN 334941-96-7 CAPLUS

CN L-Phenylalanine, N-[(2R)-2-amino-3-phenylpropyl]-N2-([1,4'-bipiperidin]-1'-ylacetyl)-D-.alpha.-asparaginyl-L-tryptophyl-, (3.fwdarw.1)-lactam (9CI)  
(CA INDEX NAME)

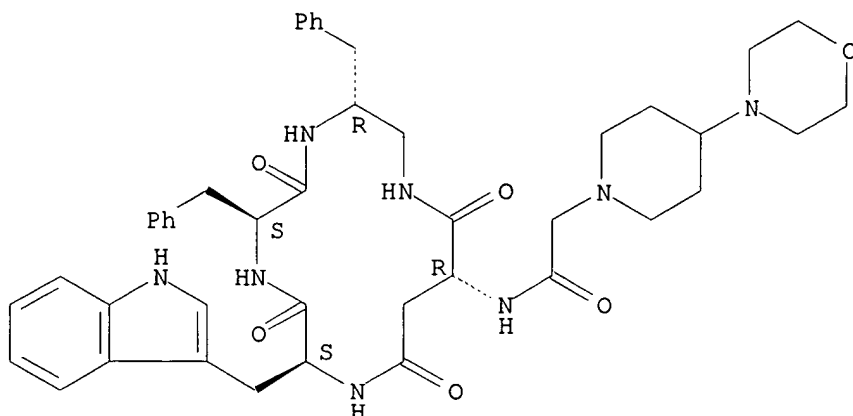
Absolute stereochemistry.



RN 334941-97-8 CAPLUS

CN L-Phenylalanine, N-[(2R)-2-amino-3-phenylpropyl]-N2-[[4-(4-morpholinyl)-1-piperidinyl]acetyl]-D-.alpha.-asparaginyl-L-tryptophyl-, (3.fwdarw.1)-lactam (9CI) (CA INDEX NAME)

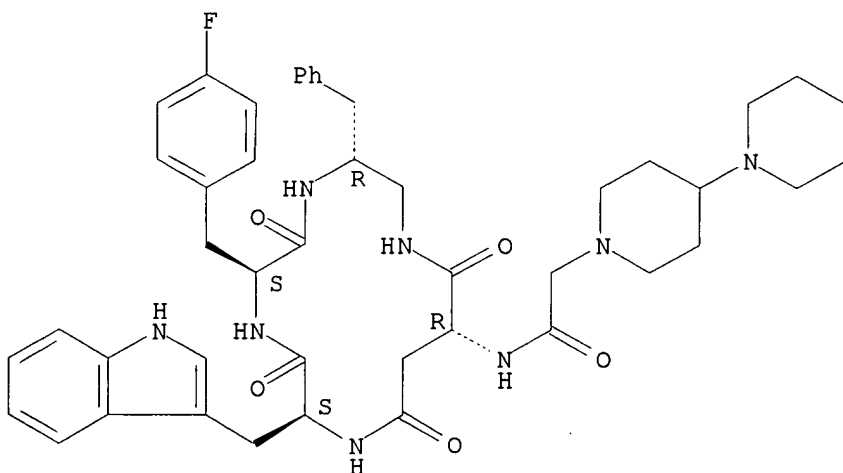
Absolute stereochemistry.



RN 334941-98-9 CAPLUS

CN L-Phenylalanine, N-[(2R)-2-amino-3-phenylpropyl]-N2-([1,4'-bipiperidin]-1'-ylacetyl)-D-.alpha.-asparaginyl-L-tryptophyl-4-fluoro-, (3.fwdarw.1)-lactam (9CI) (CA INDEX NAME)

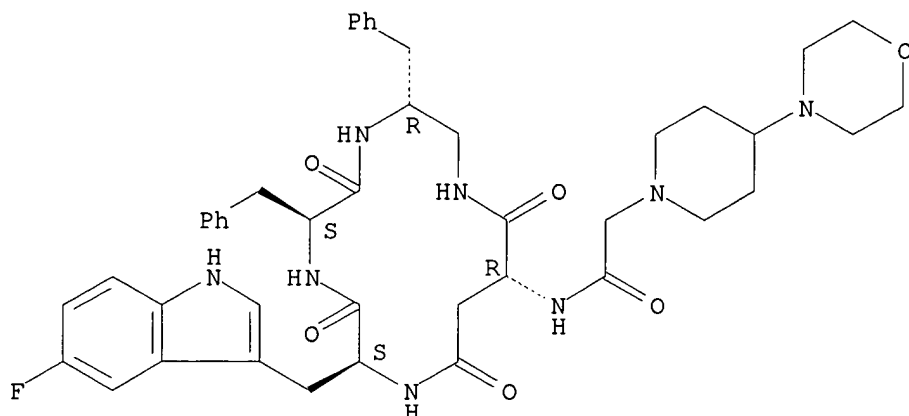
Absolute stereochemistry.



RN 334941-99-0 CAPLUS

CN L-Phenylalanine, N-[(2R)-2-amino-3-phenylpropyl]-N2-[[4-(4-morpholinyl)-1-piperidinyl]acetyl]-D-.alpha.-asparaginyl-5-fluoro-L-tryptophyl-, (3.fwdarw.1)-lactam (9CI) (CA INDEX NAME)

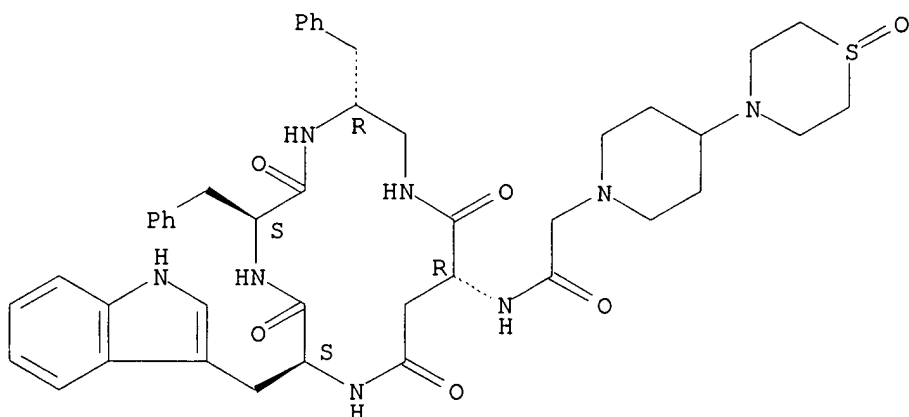
Absolute stereochemistry.



RN 334942-00-6 CAPLUS

CN L-Phenylalanine, N-[(2R)-2-amino-3-phenylpropyl]-N2-[[4-(1-oxido-4-thiomorpholinyl)-1-piperidinyl]acetyl]-D-.alpha.-asparaginyl-L-tryptophyl-, (3.fwdarw.1)-lactam (9CI) (CA INDEX NAME)

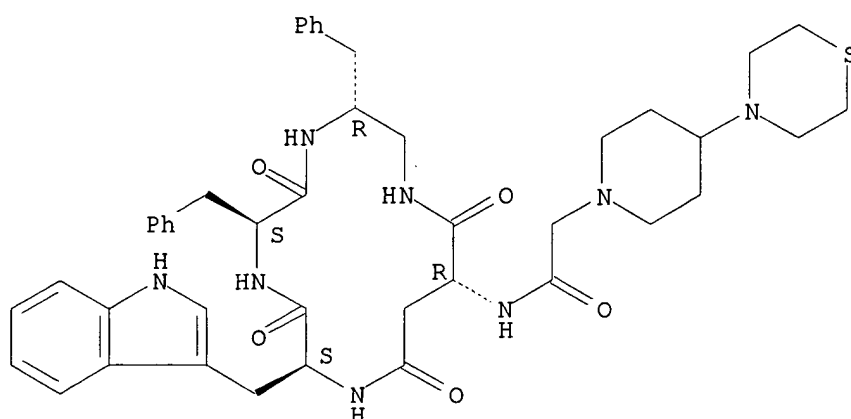
Absolute stereochemistry.



RN 334942-01-7 CAPLUS

CN L-Phenylalanine, N-[(2R)-2-amino-3-phenylpropyl]-N2-[[4-(4-thiomorpholinyl)-1-piperidinyl]acetyl]-D-.alpha.-asparaginyl-L-tryptophyl-, (3.fwdarw.1)-lactam (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 211689-26-8P 258530-43-7P

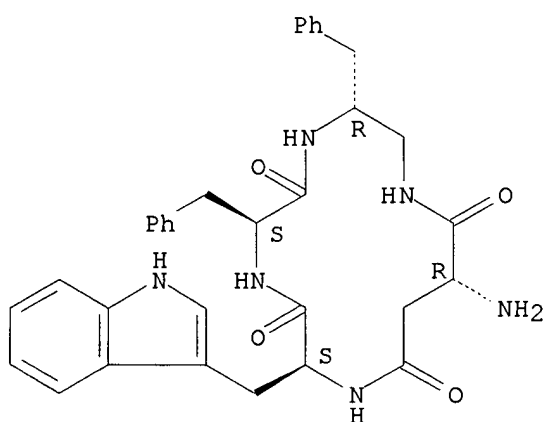
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of basic monocyclic compds. having NK2 antagonist action)

RN 211689-26-8 CAPLUS

CN L-Phenylalanine, N-[(2R)-2-amino-3-phenylpropyl]-D-.alpha.-asparaginyl-L-tryptophyl-, (3S,4S)-lactam (9CI) (CA INDEX NAME)

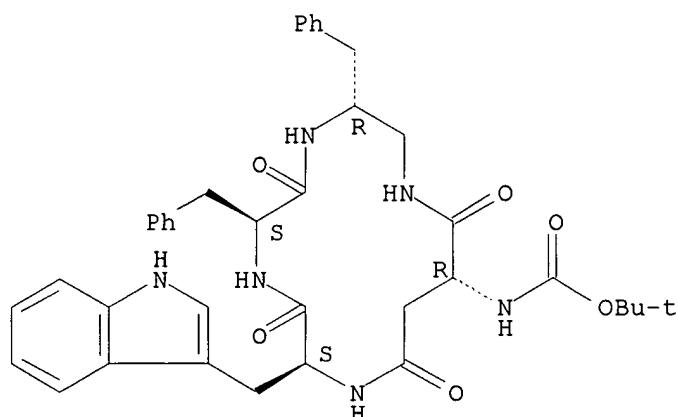
Absolute stereochemistry.



RN 258530-43-7 CAPLUS

CN L-Phenylalanine, N-[(2R)-2-amino-3-phenylpropyl]-N2-[(1,1-dimethylethoxy)carbonyl]-D-.alpha.-asparaginyl-L-tryptophyl-, (3S,4S)-lactam (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **334942-06-2P**

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of basic monocyclic compds. having NK2 antagonist action)

RN 334942-06-2 CAPLUS

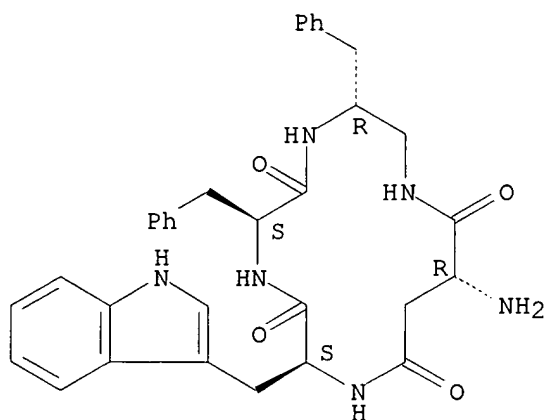
CN L-Phenylalanine, N-[(2R)-2-amino-3-phenylpropyl]-D-.alpha.-asparaginyl-L-tryptophyl-, (3.fwdarw.11)-lactam, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 211689-26-8

CMF C33 H36 N6 O4

Absolute stereochemistry.

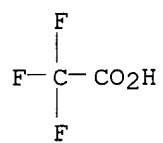


CM 2

CRN 76-05-1

CMF C2 H F3 O2

09/762,522



L22 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2002 ACS

AN 2000:117071 CAPLUS

DN 132:166521

TI Preparation of monocyclic compounds having NK-2 antagonist action

IN Altamura, Maria; Criscuoli, Marco; Guidi, Antonio; Perrotta, Enzo; Maggi, Carlo Alberto

PA Menarini Ricerche S.p.A., Italy

SO PCT Int. Appl., 50 pp.

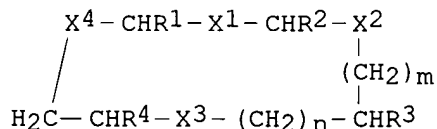
CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

PATENT NO.                      KIND      DATE                      APPLICATION NO.      DATE  
 -----  
 PI    WO 2000008046              A1      20000217              WO 1999-EP5459      19990730  
       W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ,  
          DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS,  
          JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK,  
          MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ,  
          TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ,  
          MD, RU, TJ, TM  
       RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK,  
          ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG,  
          CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG  
       IT 1304888              B1      20010405              IT 1998-FI186      19980805  
       AU 9955079              A1      20000228              AU 1999-55079      19990730  
       EP 1102789              A1      20010530              EP 1999-941479      19990730  
       R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,  
          IE, SI, LT, LV, FI, RO  
 PRAI IT 1998-FI186              A      19980805  
       WO 1999-EP5459              W      19990730  
 OS    MARPAT 132:166521  
 GI



I

AB Cyclic peptides I [X1, X2, X3, X4 = CONR, NRCO, CH2NR, NRCH2 (R = H, alkyl, benzyl); m, n = 0, 1, 2; R1, R2 = aryl, arylmethyl, 2-arylethyl; R3 = aryl, arylmethyl, 2-arylethyl; R4 = NR8R9 (R8 = H, alkyl; R9 = methanesulfonyl, tosyl, tetrahydropyranyl, tetrahydrothiopyranyl or S-oxides, piperidyl or N-substituted derivs., morpholino-, furyl- or cyanoalkyl, etc.)] or their pharmaceutically acceptable salts were prep'd. as NK-2 antagonists. Thus, cyclo{Suc[1-(4-tetrahydropyranyl)amino]-Trp-Phe-[(R)-NHCH(CH2Ph)CH2NH]} (Suc = succinyl group) was prep'd. by a multistep procedure starting from H-Trp-Phe-OH and assayed as antagonist on the NK-2 receptor of tachykinins (binding const. pKi = 8.5).

IT 258529-94-1P 258530-09-5P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT



258530-20-0P 258530-21-1P 258530-22-2P  
 258530-23-3P 258530-24-4P 258530-25-5P  
 258530-26-6P 258530-27-7P 258530-28-8P  
 258530-29-9P 258530-30-2P 258530-31-3P  
 258530-32-4P 258530-33-5P 258530-34-6P  
 258530-35-7P 258530-36-8P 258530-37-9P  
 258530-38-0P 258818-19-8P

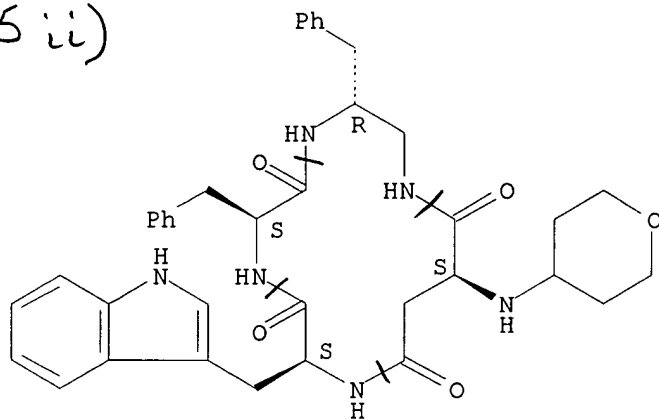
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (prepn. of monocyclic compds. having NK-2 antagonist action)

RN 258529-95-2 CAPLUS

CN L-Phenylalanine, N-[(2R)-2-amino-3-phenylpropyl]-N2-(tetrahydro-2H-pyran-4-yl)-L-.alpha.-asparaginyl-L-tryptophyl-, (3.fwdarw.1)-lactam (9CI) (CA INDEX NAME)

Absolute stereochemistry.

5 ii)

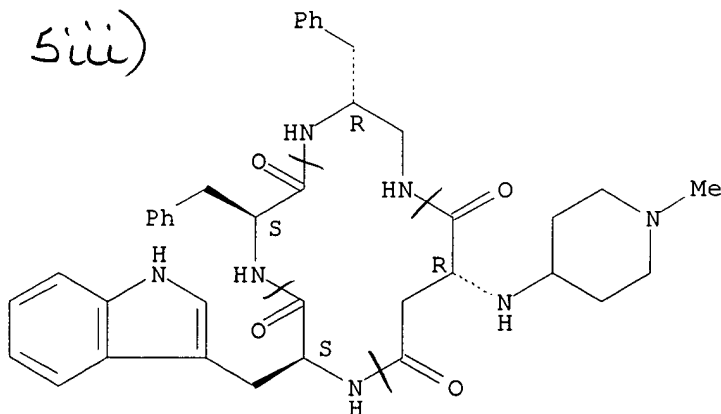


RN 258529-96-3 CAPLUS

CN L-Phenylalanine, N-[(2R)-2-amino-3-phenylpropyl]-N2-(1-methyl-4-piperidinyl)-D-.alpha.-asparaginyl-L-tryptophyl-, (3.fwdarw.1)-lactam (9CI) (CA INDEX NAME)

Absolute stereochemistry.

5 iii)

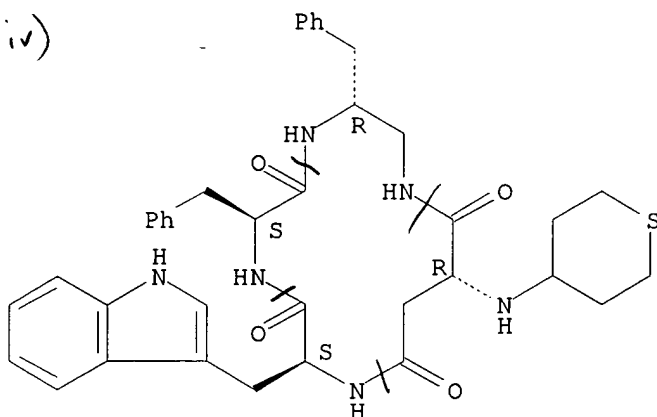


09/762,522

RN 258529-97-4 CAPLUS  
CN L-Phenylalanine, N-[(2R)-2-amino-3-phenylpropyl]-N2-(tetrahydro-2H-thiopyran-4-yl)-D-.alpha.-asparaginyll-L-tryptophyl-, (3.fwdarw.1)-lactam (9CI) (CA INDEX NAME)

Absolute stereochemistry.

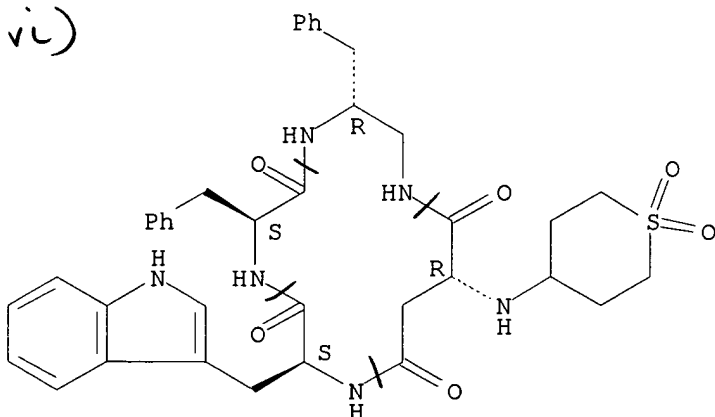
5iv)



RN 258529-98-5 CAPLUS  
CN L-Phenylalanine, N-[(2R)-2-amino-3-phenylpropyl]-N2-(tetrahydro-1,1-dioxido-2H-thiopyran-4-yl)-D-.alpha.-asparaginyll-L-tryptophyl-, (3.fwdarw.1)-lactam (9CI) (CA INDEX NAME)

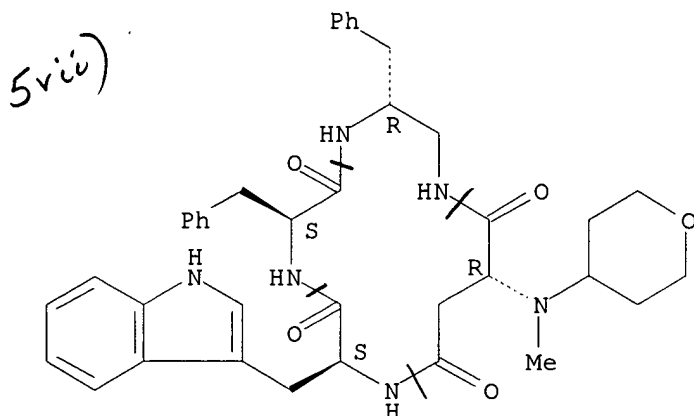
Absolute stereochemistry.

5iv)



RN 258529-99-6 CAPLUS  
CN L-Phenylalanine, N-[(2R)-2-amino-3-phenylpropyl]-N2-methyl-N2-(tetrahydro-2H-pyran-4-yl)-D-.alpha.-asparaginyll-L-tryptophyl-, (3.fwdarw.1)-lactam (9CI) (CA INDEX NAME)

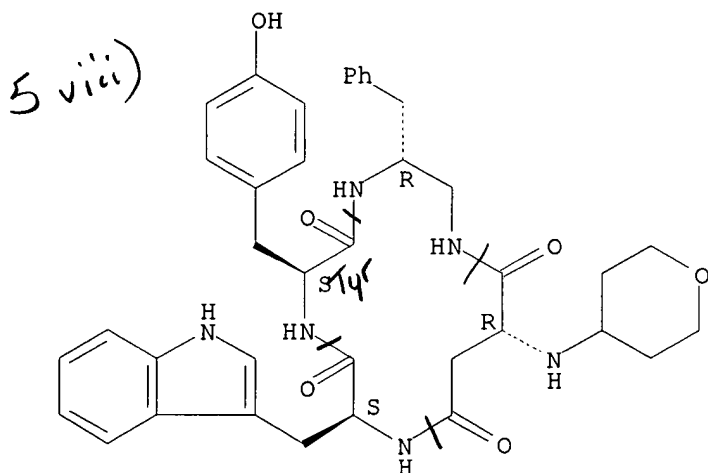
Absolute stereochemistry.



RN 258530-00-6 CAPLUS

CN L-Tyrosine, N-[(2R)-2-amino-3-phenylpropyl]-N2-(tetrahydro-2H-pyran-4-yl)-D-.alpha.-asparaginyl-L-tryptophyl-, (3.fwdarw.1)-lactam (9CI) (CA INDEX NAME)

Absolute stereochemistry.

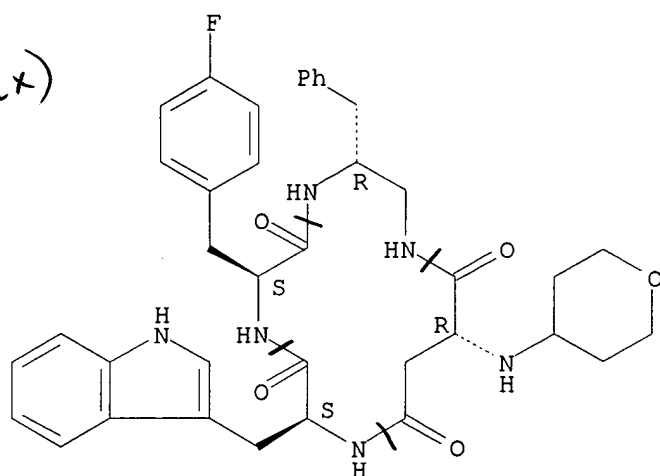


RN 258530-01-7 CAPLUS

CN L-Phenylalanine, N-[(2R)-2-amino-3-phenylpropyl]-N2-(tetrahydro-2H-pyran-4-yl)-D-.alpha.-asparaginyl-L-tryptophyl-4-fluoro-, (3.fwdarw.1)-lactam (9CI) (CA INDEX NAME)

Absolute stereochemistry.

5ix)

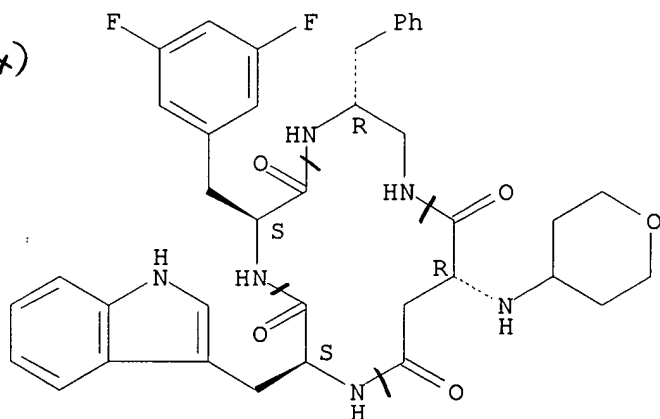


RN 258530-02-8 CAPLUS

CN L-Phenylalanine, N-[(2R)-2-amino-3-phenylpropyl]-N2-(tetrahydro-2H-pyran-4-yl)-D-.alpha.-asparaginyl-L-tryptophyl-3,5-difluoro-, (3.fwdarw.1)-lactam (9CI) (CA INDEX NAME)

Absolute stereochemistry.

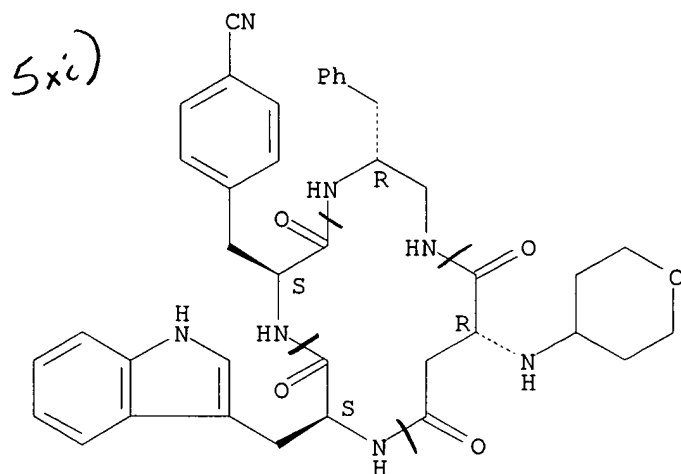
5x)



RN 258530-03-9 CAPLUS

CN L-Phenylalanine, N-[(2R)-2-amino-3-phenylpropyl]-N2-(tetrahydro-2H-pyran-4-yl)-D-.alpha.-asparaginyl-L-tryptophyl-4-cyano-, (3.fwdarw.1)-lactam (9CI) (CA INDEX NAME)

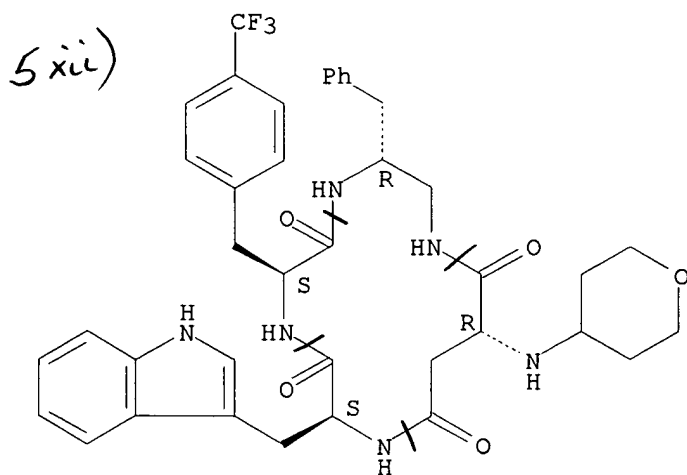
Absolute stereochemistry.



RN 258530-04-0 CAPLUS

CN L-Phenylalanine, N-[(2R)-2-amino-3-phenylpropyl]-N2-(tetrahydro-2H-pyran-4-yl)-D-.alpha.-asparaginyl-L-tryptophyl-4-(trifluoromethyl)-, (3.fwdarw.1)-lactam (9CI) (CA INDEX NAME)

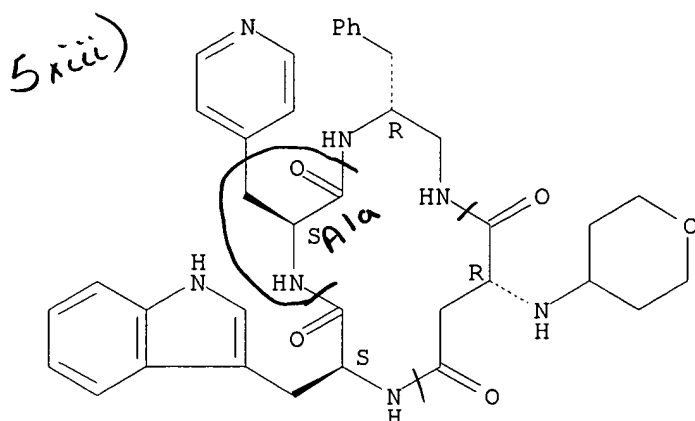
Absolute stereochemistry.



RN 258530-05-1 CAPLUS

CN L-Alanine, N-[(2R)-2-amino-3-phenylpropyl]-N2-(tetrahydro-2H-pyran-4-yl)-D-.alpha.-asparaginyl-L-tryptophyl-3-(4-pyridinyl)-, (3.fwdarw.1)-lactam (9CI) (CA INDEX NAME)

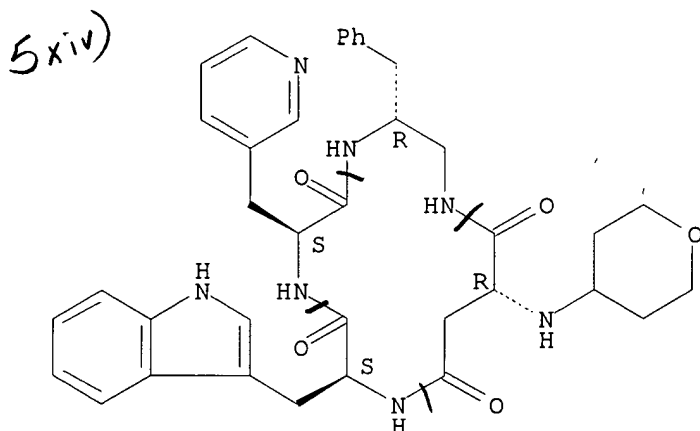
Absolute stereochemistry.



RN 258530-06-2 CAPLUS

CN L-Alanine, N-[(2R)-2-amino-3-phenylpropyl]-N2-(tetrahydro-2H-pyran-4-yl)-D-.alpha.-asparaginyl-L-tryptophyl-3-(3-pyridinyl)-, (3.fwdarw.1)-lactam  
(9CI) (CA INDEX NAME)

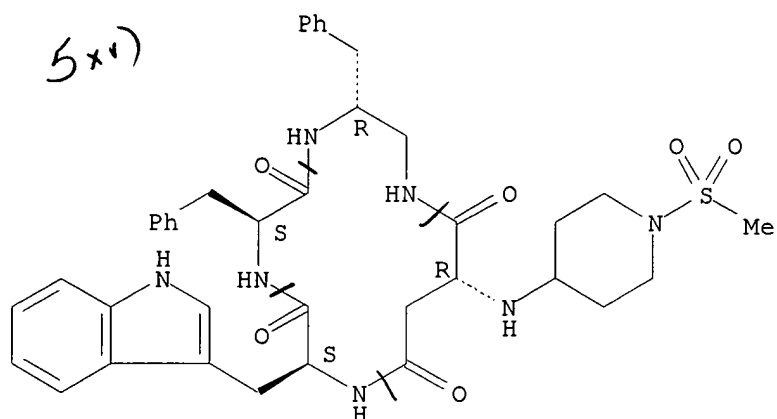
Absolute stereochemistry.



RN 258530-07-3 CAPLUS

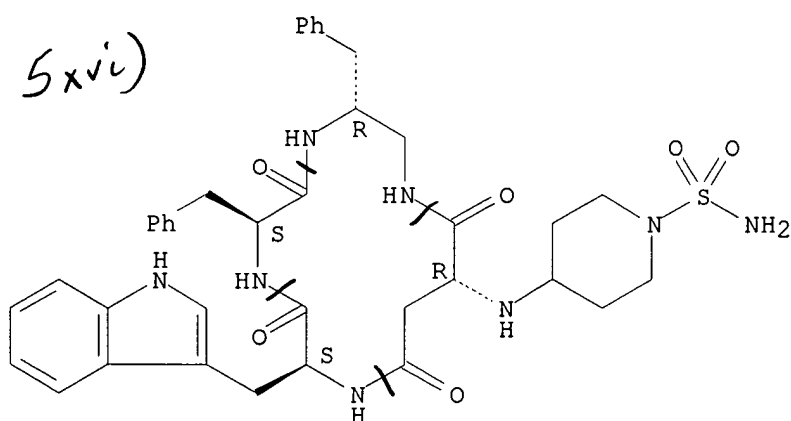
CN L-Phenylalanine, N-[(2R)-2-amino-3-phenylpropyl]-N2-[1-(methylsulfonyl)-4-piperidinyl]-D-.alpha.-asparaginyl-L-tryptophyl-, (3.fwdarw.1)-lactam  
(9CI) (CA INDEX NAME)

Absolute stereochemistry.



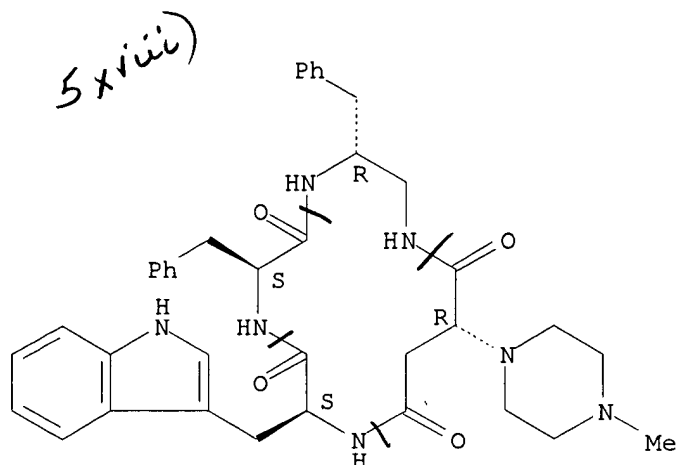
RN 258530-08-4 CAPLUS  
 CN L-Phenylalanine, N-[(2R)-2-amino-3-phenylpropyl]-N2-[1-(aminosulfonyl)-4-piperidinyl]-D-.alpha.-asparaginyl-L-tryptophyl-, (3.fwdarw.1)-lactam  
 (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 258530-10-8 CAPLUS  
 CN Cyclo[L-phenylalanyl-(.beta.R)-.beta.-[[[(2R)-2-amino-3-phenylpropyl]amino]carbonyl]-4-methyl-1-piperazinepropanoyl-L-tryptophyl]  
 (9CI) (CA INDEX NAME)

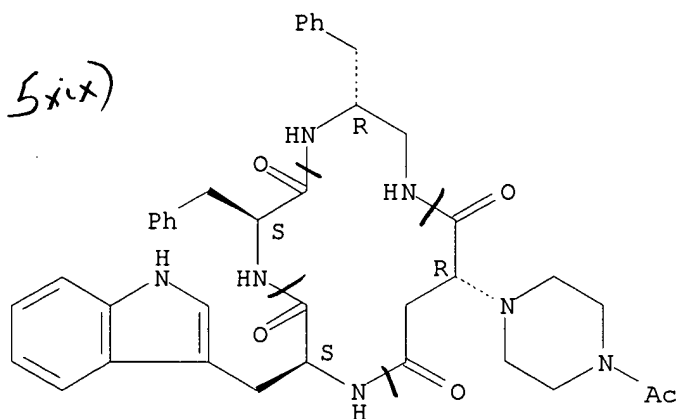
Absolute stereochemistry.



RN 258530-11-9 CAPLUS

CN Cyclo[L-phenylalanyl-(.beta.R)-4-acetyl-.beta.-[[[(2R)-2-amino-3-phenylpropyl]amino]carbonyl]-1-piperazinepropanoyl-L-tryptophyl] (9CI)  
(CA INDEX NAME)

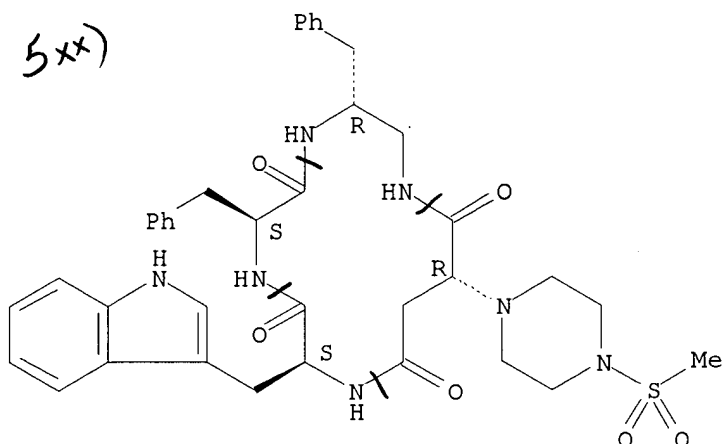
Absolute stereochemistry.



RN 258530-12-0 CAPLUS

CN Cyclo[L-phenylalanyl-(.beta.R)-.beta.-[[[(2R)-2-amino-3-phenylpropyl]amino]carbonyl]-4-(methylsulfonyl)-1-piperazinepropanoyl-L-tryptophyl] (9CI) (CA INDEX NAME)

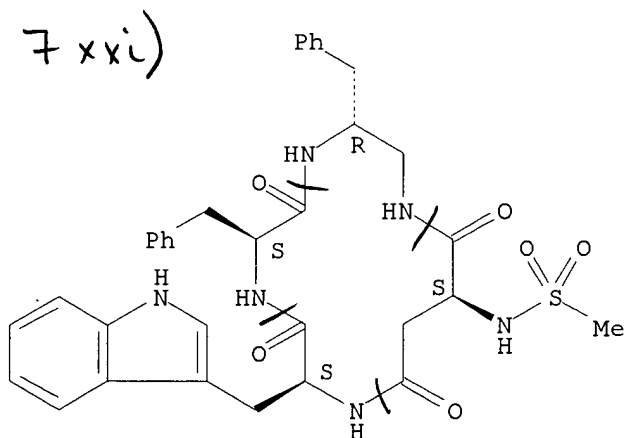
Absolute stereochemistry.



RN 258530-13-1 CAPLUS

CN L-Phenylalanine, N-[(2R)-2-amino-3-phenylpropyl]-N2-(methylsulfonyl)-L-.alpha.-asparaginyl-L-tryptophyl-, (3.fwdarw.1)-lactam (9CI) (CA INDEX NAME)

Absolute stereochemistry.

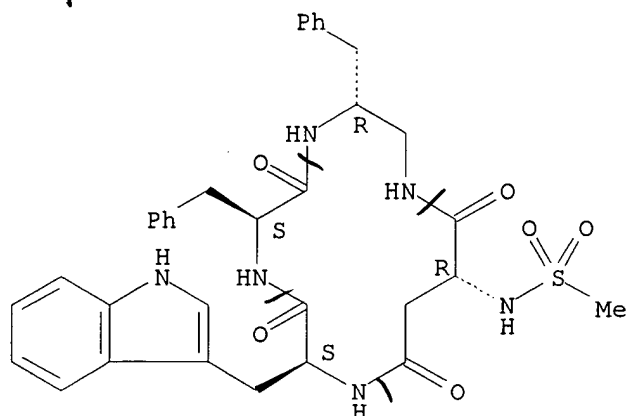


RN 258530-14-2 CAPLUS

CN L-Phenylalanine, N-[(2R)-2-amino-3-phenylpropyl]-N2-(methylsulfonyl)-D-.alpha.-asparaginyl-L-tryptophyl-, (3.fwdarw.1)-lactam (9CI) (CA INDEX NAME)

Absolute stereochemistry.

7 xxi)

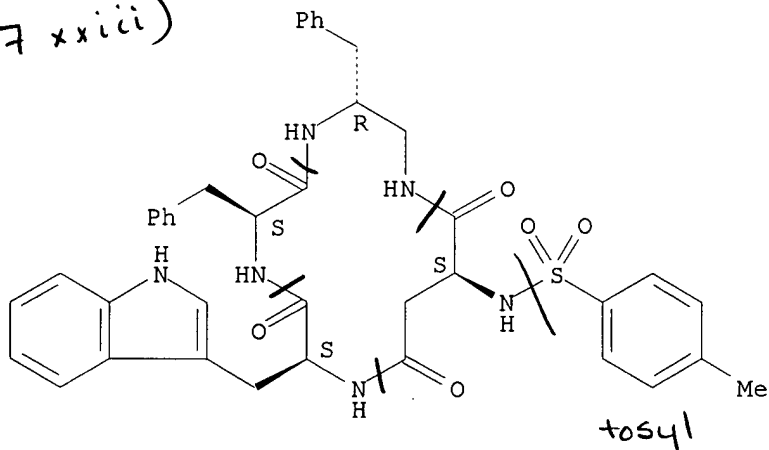


RN 258530-15-3 CAPLUS

CN L-Phenylalanine, N-[(2R)-2-amino-3-phenylpropyl]-N2-[(4-methylphenyl)sulfonyl]-L-.alpha.-asparaginyl-L-tryptophyl-, (3.fwdarw.1)-lactam (9CI) (CA INDEX NAME)

Absolute stereochemistry.

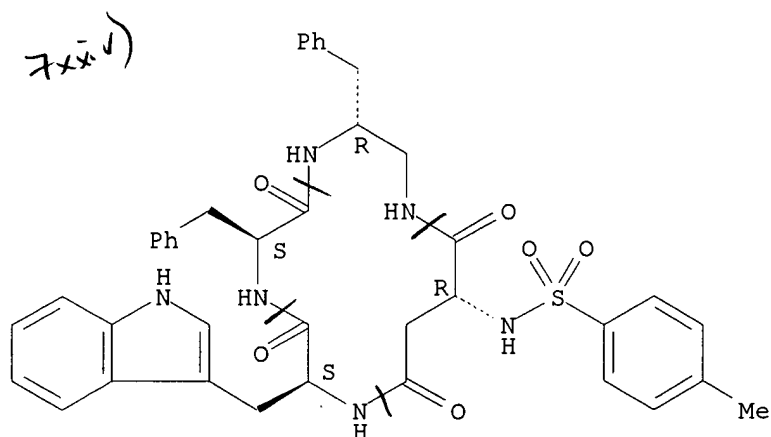
7 xxi)



RN 258530-16-4 CAPLUS

CN L-Phenylalanine, N-[(2R)-2-amino-3-phenylpropyl]-N2-[(4-methylphenyl)sulfonyl]-D-.alpha.-asparaginyl-L-tryptophyl-, (3.fwdarw.1)-lactam (9CI) (CA INDEX NAME)

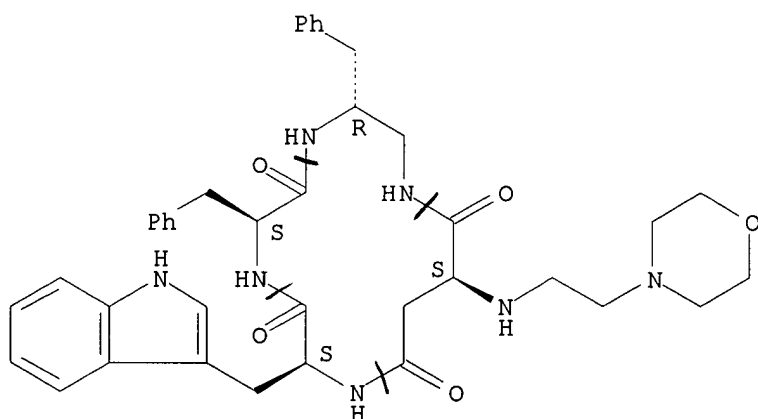
Absolute stereochemistry.



RN 258530-17-5 CAPLUS

CN L-Phenylalanine, N-[(2R)-2-amino-3-phenylpropyl]-N2-[2-(4-morpholinyl)ethyl]-L-.alpha.-asparaginyl-L-tryptophyl-, (3.fwdarw.1)-lactam (9CI) (CA INDEX NAME)

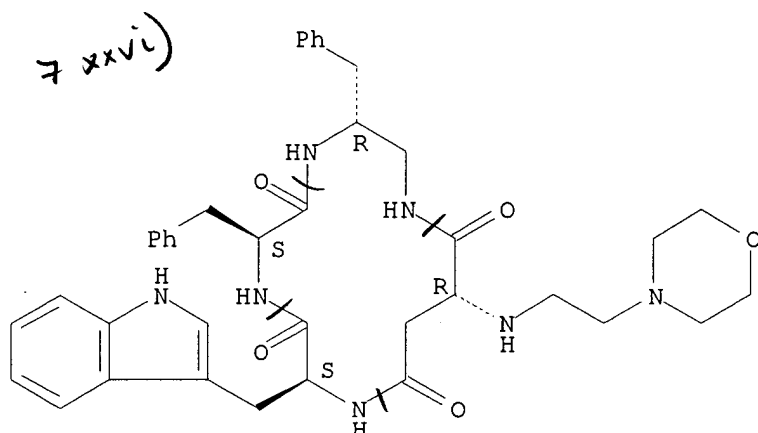
Absolute stereochemistry.



RN 258530-18-6 CAPLUS

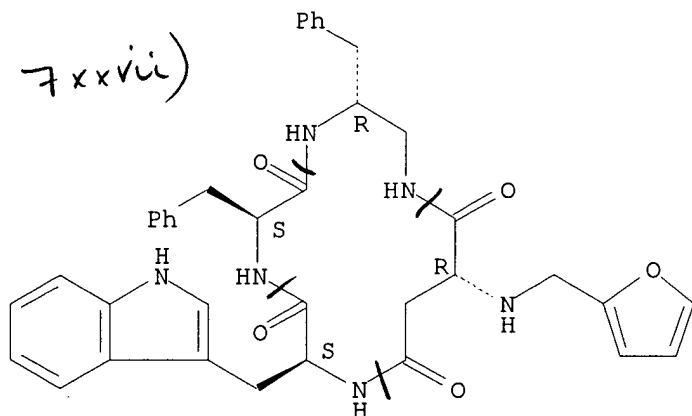
CN L-Phenylalanine, N-[(2R)-2-amino-3-phenylpropyl]-N2-[2-(4-morpholinyl)ethyl]-D-.alpha.-asparaginyl-L-tryptophyl-, (3.fwdarw.1)-lactam (9CI) (CA INDEX NAME)

Absolute stereochemistry.



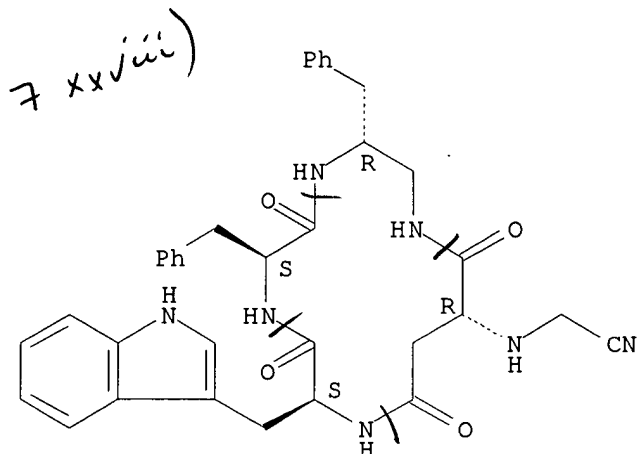
RN 258530-19-7 CAPLUS  
 CN L-Phenylalanine, N-[(2R)-2-amino-3-phenylpropyl]-N2-(2-furanylmethyl)-D-  
 .alpha.-asparaginyll-L-tryptophyl-, (3.fwdarw.1)-lactam (9CI) (CA INDEX  
 NAME)

Absolute stereochemistry.



RN 258530-20-0 CAPLUS  
 CN L-Phenylalanine, N-[(2R)-2-amino-3-phenylpropyl]-N2-(cyanomethyl)-D-  
 .alpha.-asparaginyll-L-tryptophyl-, (3.fwdarw.1)-lactam (9CI) (CA INDEX  
 NAME)

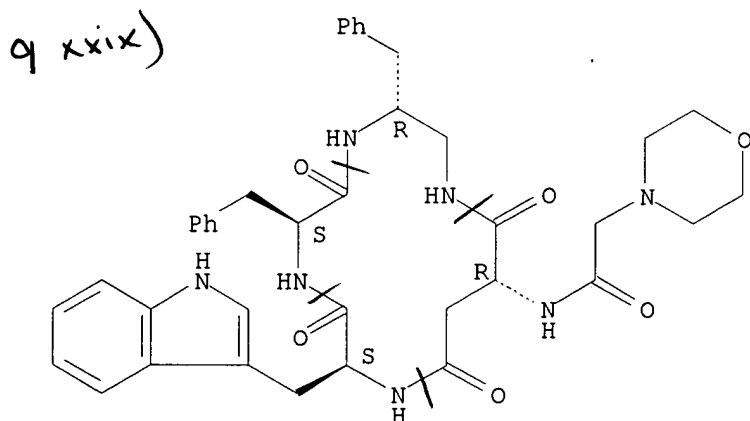
Absolute stereochemistry.



RN 258530-21-1 CAPLUS

CN L-Phenylalanine, N-[(2R)-2-amino-3-phenylpropyl]-N2-(4-morpholinylacetyl)-D-.alpha.-asparaginyl-L-tryptophyl-, (3.fwdarw.1)-lactam (9CI) (CA INDEX NAME)

Absolute stereochemistry.

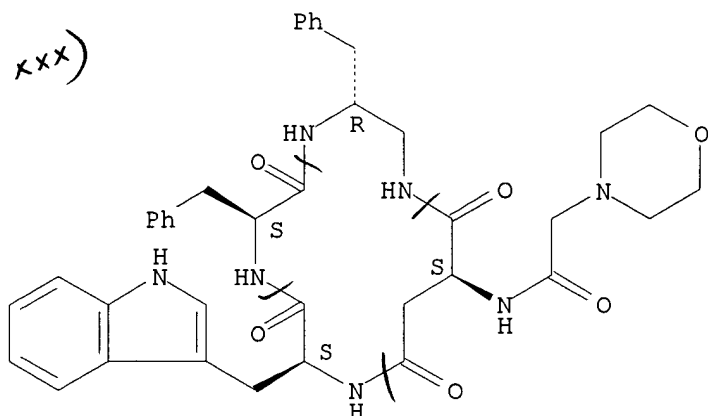


RN 258530-22-2 CAPLUS

CN L-Phenylalanine, N-[(2R)-2-amino-3-phenylpropyl]-N2-(4-morpholinylacetyl)-L-.alpha.-asparaginyl-L-tryptophyl-, (3.fwdarw.1)-lactam (9CI) (CA INDEX NAME)

Absolute stereochemistry.

9xxx)

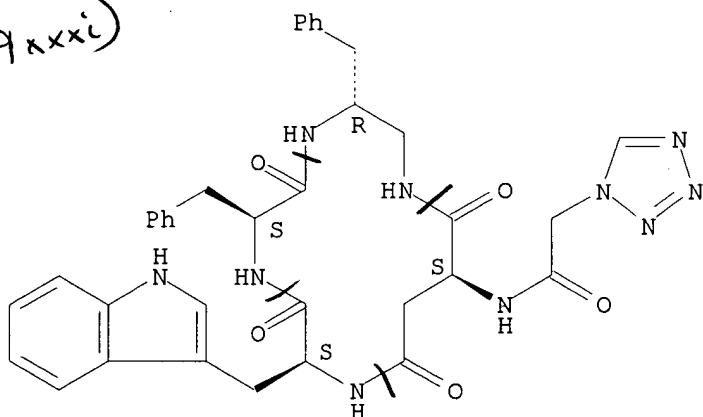


RN 258530-23-3 CAPLUS

CN L-Phenylalanine, N-[(2R)-2-amino-3-phenylpropyl]-N2-(1H-tetrazol-1-ylacetyl)-L-.alpha.-asparaginyl-L-tryptophyl-, (3.fwdarw.1)-lactam (9CI)  
(CA INDEX NAME)

Absolute stereochemistry.

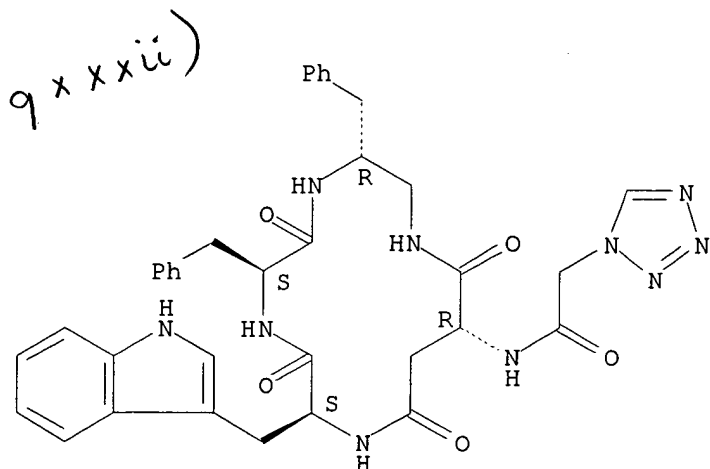
9xxxi)



RN 258530-24-4 CAPLUS

CN L-Phenylalanine, N-[(2R)-2-amino-3-phenylpropyl]-N2-(1H-tetrazol-1-ylacetyl)-D-.alpha.-asparaginyl-L-tryptophyl-, (3.fwdarw.1)-lactam (9CI)  
(CA INDEX NAME)

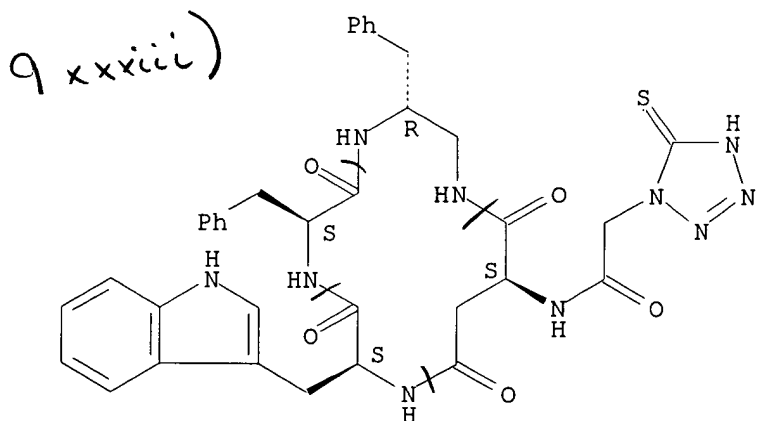
Absolute stereochemistry.



RN 258530-25-5 CAPLUS

CN L-Phenylalanine, N-[(2R)-2-amino-3-phenylpropyl]-N2-[(2,5-dihydro-5-thioxo-1H-tetrazol-1-yl)acetyl]-L-.alpha.-asparaginyl-L-tryptophyl-, (3.fwdarw.1)-lactam (9CI) (CA INDEX NAME)

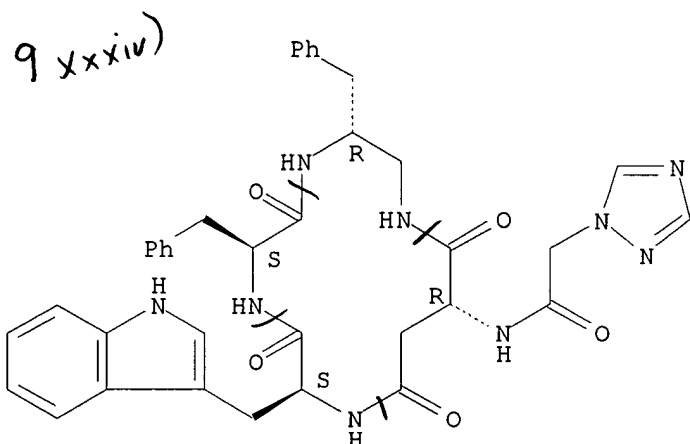
Absolute stereochemistry.



RN 258530-26-6 CAPLUS

CN L-Phenylalanine, N-[(2R)-2-amino-3-phenylpropyl]-N2-(1H-1,2,4-triazol-1-ylacetyl)-D-.alpha.-asparaginyl-L-tryptophyl-, (3.fwdarw.1)-lactam (9CI) (CA INDEX NAME)

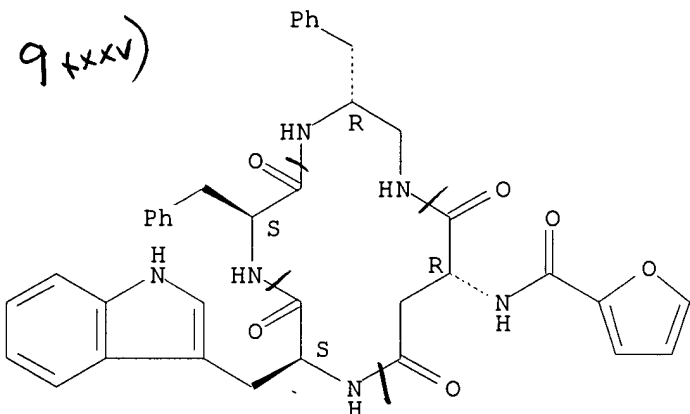
Absolute stereochemistry.



RN 258530-27-7 CAPLUS

CN L-Phenylalanine, N-[(2R)-2-amino-3-phenylpropyl]-N2-(2-furanylcarbonyl)-D-.alpha.-asparaginyl-L-tryptophyl-, (3.fwdarw.1)-lactam (9CI) (CA INDEX NAME)

Absolute stereochemistry.

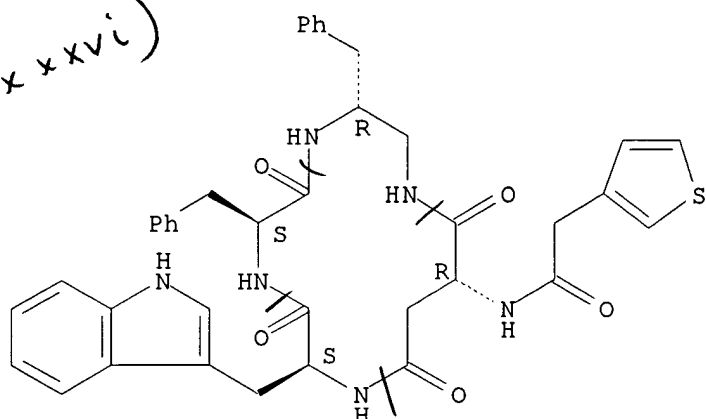


RN 258530-28-8 CAPLUS

CN L-Phenylalanine, N-[(2R)-2-amino-3-phenylpropyl]-N2-(3-thienylacetyl)-D-.alpha.-asparaginyl-L-tryptophyl-, (3.fwdarw.1)-lactam (9CI) (CA INDEX NAME)

Absolute stereochemistry.

9xxxvi)

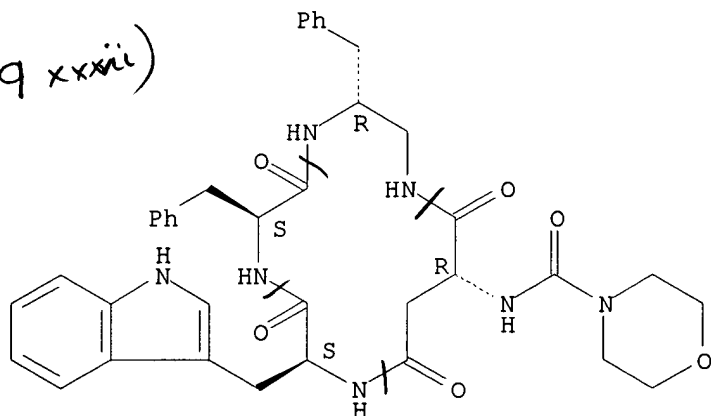


RN 258530-29-9 CAPLUS

CN L-Phenylalanine, N-[(2R)-2-amino-3-phenylpropyl]-N2-(4-morpholinylcarbonyl)-D-.alpha.-asparaginyl-L-tryptophyl-, (3.fwdarw.1)-lactam (9CI) (CA INDEX NAME)

Absolute stereochemistry.

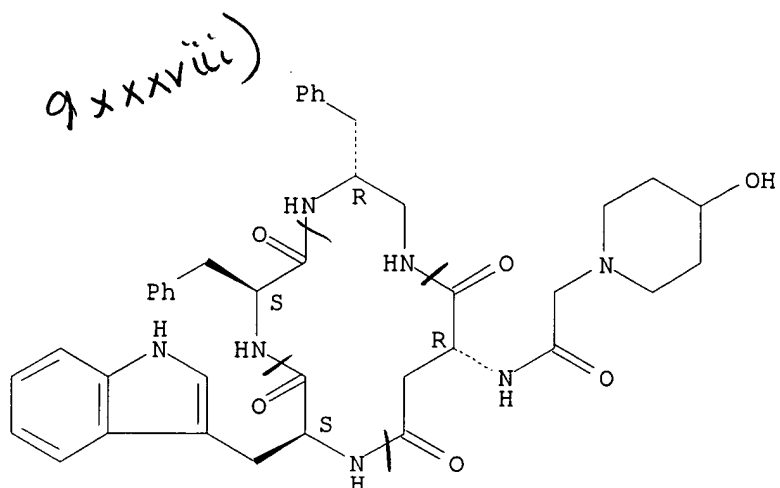
9xxxii)



RN 258530-30-2 CAPLUS

CN L-Phenylalanine, N-[(2R)-2-amino-3-phenylpropyl]-N2-[(4-hydroxy-1-piperidinyl)acetyl]-D-.alpha.-asparaginyl-L-tryptophyl-, (3.fwdarw.1)-lactam (9CI) (CA INDEX NAME)

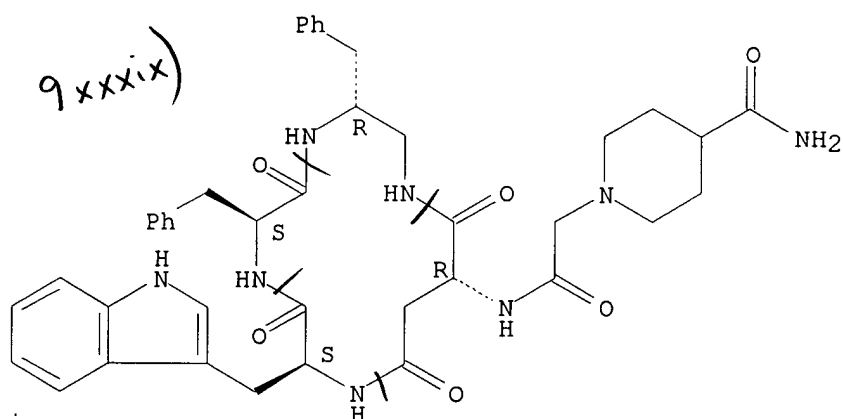
Absolute stereochemistry.



RN 258530-31-3 CAPLUS

CN L-Phenylalanine, N2-[[4-(aminocarbonyl)-1-piperidinyl]acetyl]-N-[(2R)-2-amino-3-phenylpropyl]-D-.alpha.-asparaginyl-L-tryptophyl-,  
(3.fwdarw.1)-lactam (9CI) (CA INDEX NAME)

Absolute stereochemistry.

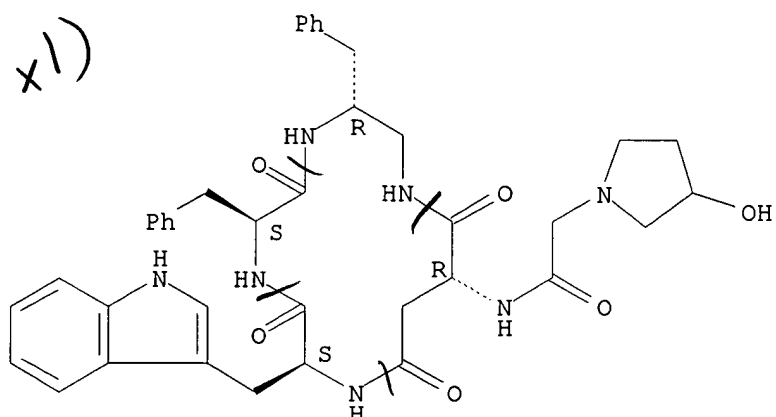


RN 258530-32-4 CAPLUS

CN L-Phenylalanine, N-[(2R)-2-amino-3-phenylpropyl]-N2-[(3-hydroxy-1-pyrrolidinyl)acetyl]-D-.alpha.-asparaginyl-L-tryptophyl-,  
(3.fwdarw.1)-lactam (9CI) (CA INDEX NAME)

Absolute stereochemistry.

9 x 1)

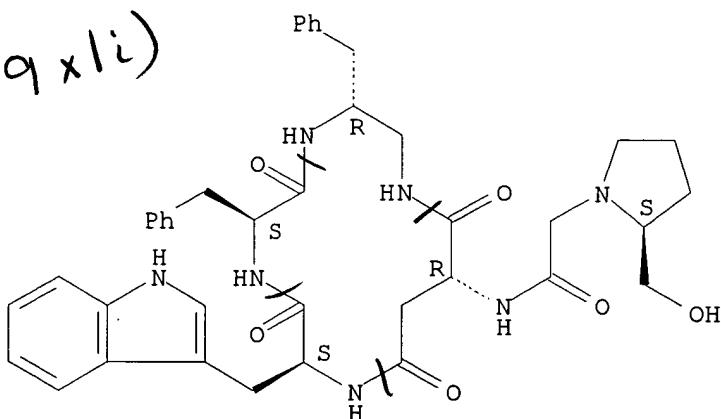


RN 258530-33-5 CAPLUS

CN L-Phenylalanine, N-[(2R)-2-amino-3-phenylpropyl]-N2-[(2S)-2-(hydroxymethyl)-1-pyrrolidinyl]acetyl]-D-.alpha.-asparaginyl-L-tryptophyl-, (3.fwdarw.1)-lactam (9CI) (CA INDEX NAME)

Absolute stereochemistry.

9 x 1i)

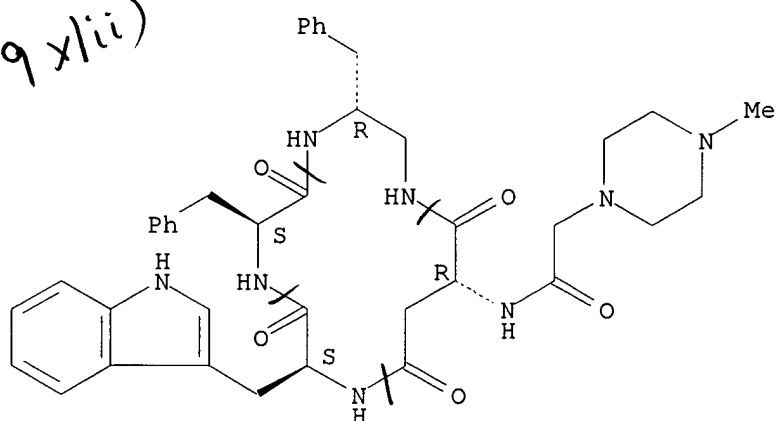


RN 258530-34-6 CAPLUS

CN L-Phenylalanine, N-[(2R)-2-amino-3-phenylpropyl]-N2-[(4-methyl-1-piperazinyl)acetyl]-D-.alpha.-asparaginyl-L-tryptophyl-, (3.fwdarw.1)-lactam (9CI) (CA INDEX NAME)

Absolute stereochemistry.

9x/ii)

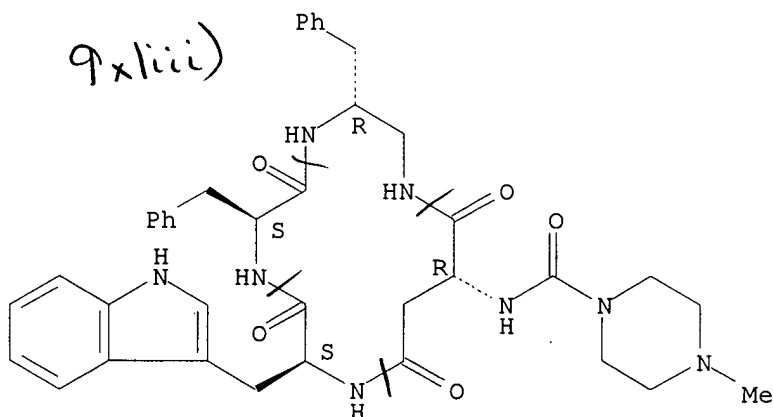


RN 258530-35-7 CAPLUS

CN L-Phenylalanine, N-[(2R)-2-amino-3-phenylpropyl]-N2-[(4-methyl-1-piperazinyl)carbonyl]-D-.alpha.-asparaginyl-L-tryptophyl-, (3.fwdarw.1)-lactam (9CI) (CA INDEX NAME)

Absolute stereochemistry.

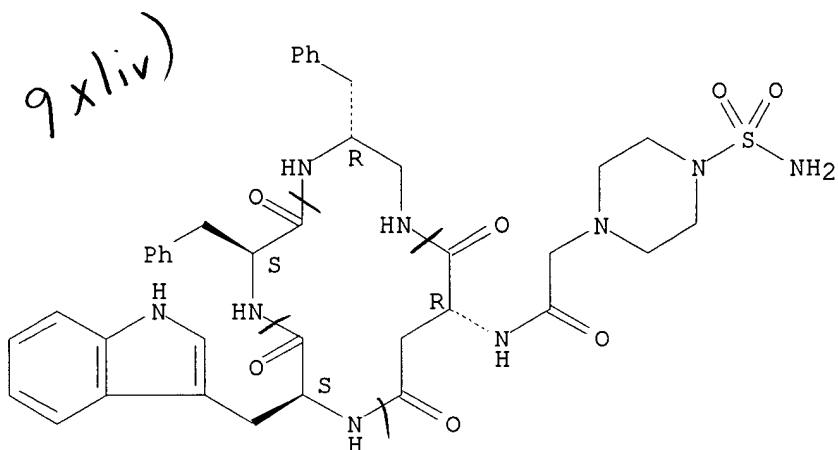
9x/iii)



RN 258530-36-8 CAPLUS

CN L-Phenylalanine, N-[(2R)-2-amino-3-phenylpropyl]-N2-[[4-(aminosulfonyl)-1-piperazinyl]acetyl]-D-.alpha.-asparaginyl-L-tryptophyl-, (3.fwdarw.1)-lactam (9CI) (CA INDEX NAME)

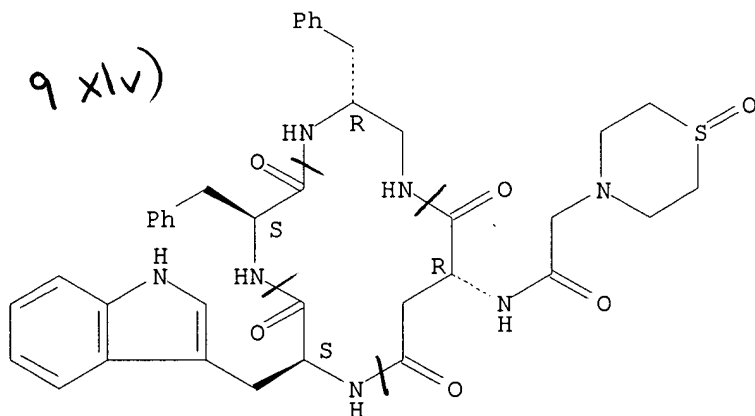
Absolute stereochemistry.



RN 258530-37-9 CAPLUS

CN L-Phenylalanine, N-[(2R)-2-amino-3-phenylpropyl]-N2-[(1-oxido-4-thiomorpholinyl)acetyl]-D-.alpha.-asparaginyl-L-tryptophyl-, (3.fwdarw.1)-lactam (9CI) (CA INDEX NAME)

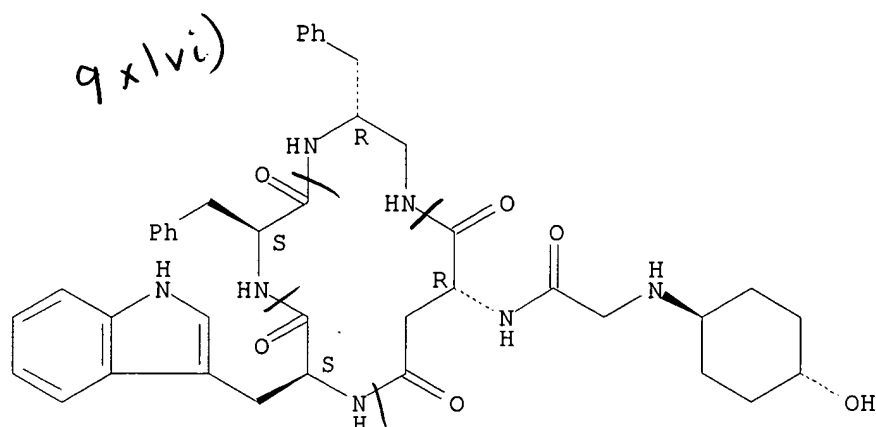
Absolute stereochemistry.



RN 258530-38-0 CAPLUS

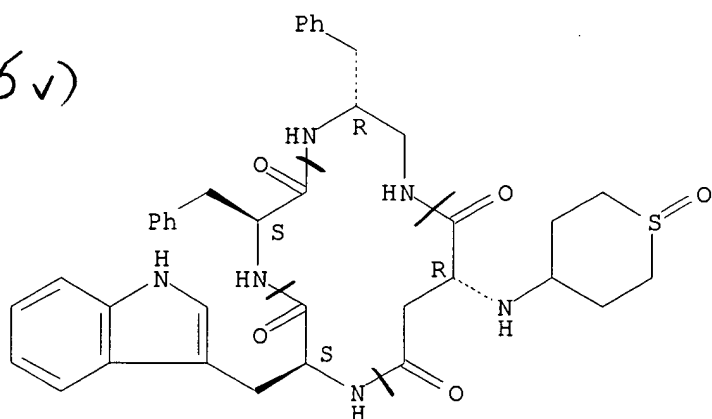
CN L-Phenylalanine, N-(trans-4-hydroxycyclohexyl)glycyl-N-[(2R)-2-amino-3-phenylpropyl]-D-.alpha.-asparaginyl-L-tryptophyl-, (4.fwdarw.2)-lactam (9CI) (CA INDEX NAME)

Absolute stereochemistry.



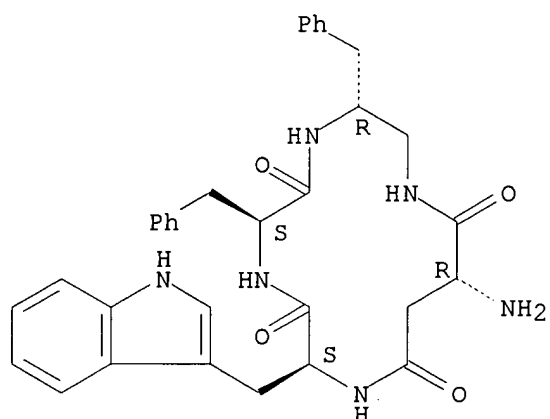
RN 258818-19-8 CAPLUS  
 CN L-Phenylalanine, N-[(2R)-2-amino-3-phenylpropyl]-N2-(tetrahydro-1-oxido-2H-thiopyran-4-yl)-D-.alpha.-asparaginyl-L-tryptophyl-, (3.fwdarw.1)-lactam (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 211689-26-8P 211689-75-7P 258530-43-7P  
 258530-64-2P 258530-65-3P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (prepn. of monocyclic compds. having NK-2 antagonist action)  
 RN 211689-26-8 CAPLUS  
 CN L-Phenylalanine, N-[(2R)-2-amino-3-phenylpropyl]-D-.alpha.-asparaginyl-L-tryptophyl-, (3.fwdarw.11)-lactam (9CI) (CA INDEX NAME)

Absolute stereochemistry.

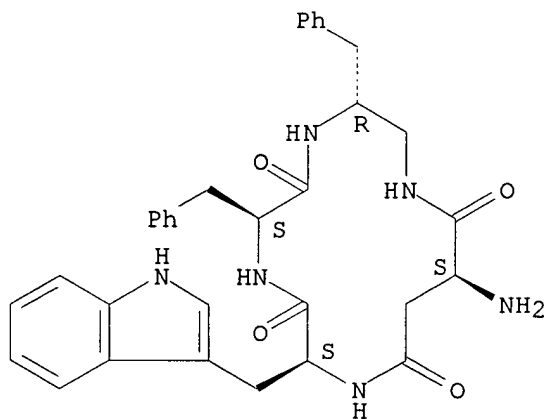


RN 211689-75-7 CAPLUS  
 CN L-Phenylalanine, N-[(2R)-2-amino-3-phenylpropyl]-L-.alpha.-asparaginyl-L-tryptophyl-, (3S,4S)-lactam, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 211689-25-7  
 CMF C33 H36 N6 O4

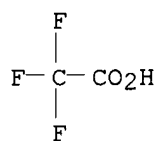
Absolute stereochemistry.



CM 2

CRN 76-05-1  
 CMF C2 H F3 O2

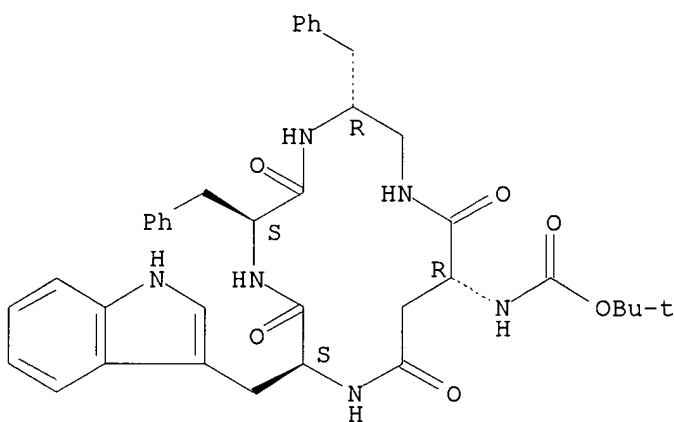
09/762,522



RN 258530-43-7 CAPLUS

CN L-Phenylalanine, N-[(2R)-2-amino-3-phenylpropyl]-N2-[(1,1-dimethylethoxy)carbonyl]-D-.alpha.-asparaginy-L-tryptophyl-, (3.fwdarw.1)-lactam (9CI) (CA INDEX NAME)

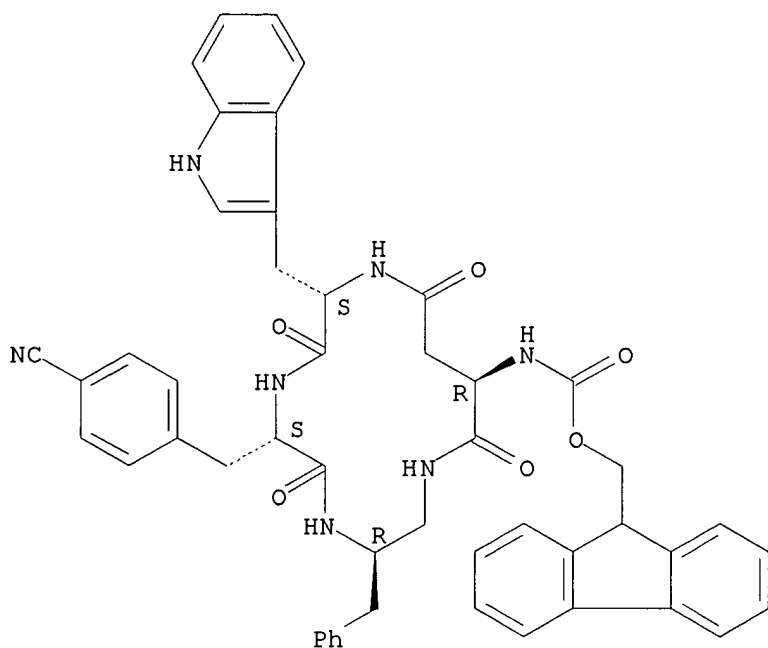
Absolute stereochemistry.



RN 258530-64-2 CAPLUS

CN L-Phenylalanine, N-[(2R)-2-amino-3-phenylpropyl]-N2-[(9H-fluoren-9-ylmethoxy)carbonyl]-D-.alpha.-asparaginy-L-tryptophyl-4-cyano-, (3.fwdarw.1)-lactam (9CI) (CA INDEX NAME)

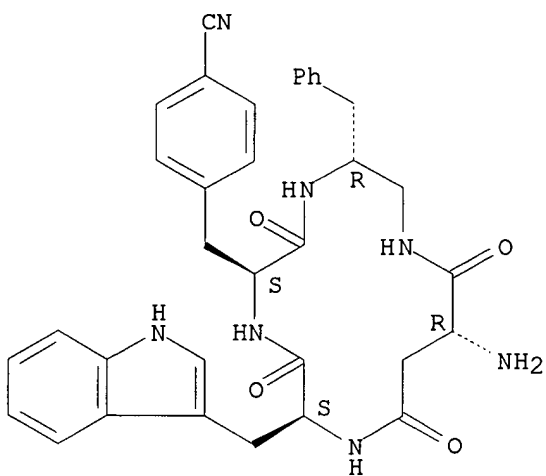
Absolute stereochemistry.



RN 258530-65-3 CAPLUS

CN L-Phenylalanine, N-[(2R)-2-amino-3-phenylpropyl]-D-.alpha.-asparaginyl-L-tryptophyl-4-cyano-, (3.fwdarw.1)-lactam (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RE.CNT 7

THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2002 ACS

AN 1998:550436 CAPLUS

DN 129:189672

TI Monocyclic compounds with four bifunctional residues having NK-2 antagonist action

IN Giorgi, Raffaello; Di Bugno, Cristina; Giannotti, Danilo; Maggi, Carlo Alberto

PA Menarini Ricerche S.p.A., Italy

SO PCT Int. Appl., 39 pp.

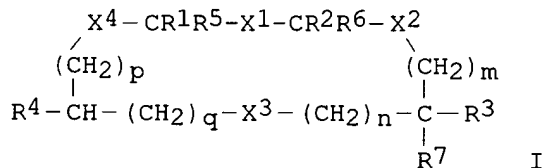
CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9834949	A2	19980813	WO 1998-EP599	19980204
	WO 9834949	A3	19981022		
	W:	AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
	RW:	GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG			
	AU 9866201	A1	19980826	AU 1998-66201	19980204
	EP 1017711	A2	20000712	EP 1998-908055	19980204
	R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, NL, SE, PT, IE, FI			
	JP 2001511167	T2	20010807	JP 1998-533751	19980204
	ZA 9800931	A	19980807	ZA 1998-931	19980205
PRAI	IT 1997-FI20	A	19970207		
	WO 1998-EP599	W	19980204		
OS	MARPAT 129:189672				
GI					



AB Monocyclic compds. I [X1, X2, X3, X4 = CONR, NRCO, OCO, CO2, CH2NR, NR, CH2, CH2CH2 (R = H, alkyl, benzyl); m, n, p, q = 0, 1, 2; R1, R2 = aryl, arylmethyl, 2-arylethyl; R3 = H, alkyl, aryl, arylmethyl, 2-arylethyl; R4 = H, alkyl, L-Q (L = bond or alkyl group; Q = H, OH, NH2, CO2H, tetrazolyl, SO2NH2, etc.); R5, R6, R7 = H, alkyl] or their pharmaceutically acceptable salts were prepd. as NK-2 antagonists. Thus, cyclo[-Suc-Trp-Phe-[(R)-NHCH(CH2Ph)CH2NH-]] (Suc = succinyl group) was prepd. from H-Trp-Phe-OH, (R)-1-benzyl-2-(benzyloxycarbonylamino)ethylamine, and succinic anhydride. The synthesized compds. were assayed as human NK-2 receptor antagonists.

IT 211689-25-7P 211689-26-8P 211689-49-5P

**211689-52-0P**

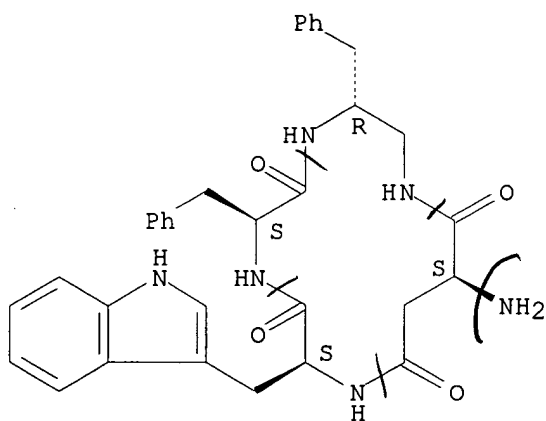
RL: BAC (Biological activity or effector, except adverse); RCT (Reactant);  
 SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological  
 study); PREP (Preparation); USES (Uses)

(monocyclic compds. with four bifunctional residues having NK-2  
 antagonist action)

RN 211689-25-7 CAPLUS

CN L-Phenylalanine, N-[(2R)-2-amino-3-phenylpropyl]-L-.alpha.-asparaginyl-L-  
 tryptophyl-, (3.fwdarw.1)-lactam (9CI) (CA INDEX NAME)

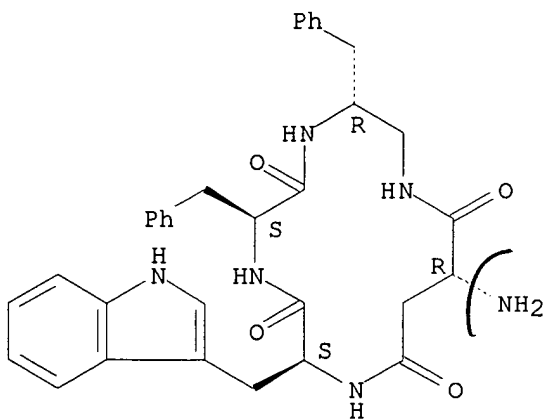
Absolute stereochemistry.



RN 211689-26-8 CAPLUS

CN L-Phenylalanine, N-[(2R)-2-amino-3-phenylpropyl]-D-.alpha.-asparaginyl-L-  
 tryptophyl-, (3.fwdarw.11)-lactam (9CI) (CA INDEX NAME)

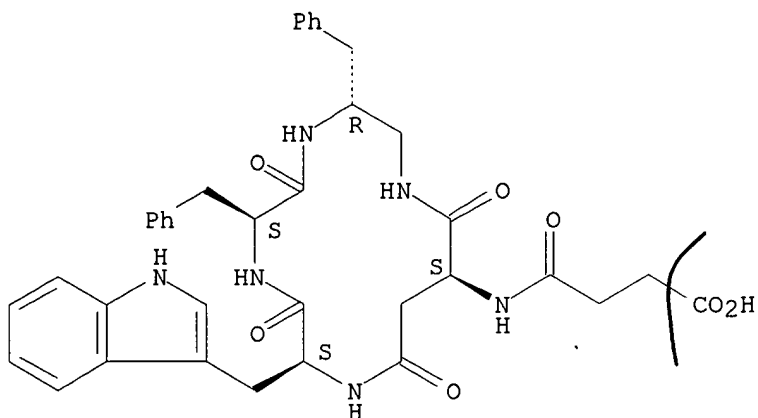
Absolute stereochemistry.



RN 211689-49-5 CAPLUS

CN L-Phenylalanine, N-[(2R)-2-amino-3-phenylpropyl]-N2-(3-carboxy-1-  
 oxopropyl)-L-.alpha.-asparaginyl-L-tryptophyl-, (3.fwdarw.1)-lactam (9CI)  
 (CA INDEX NAME)

Absolute stereochemistry.

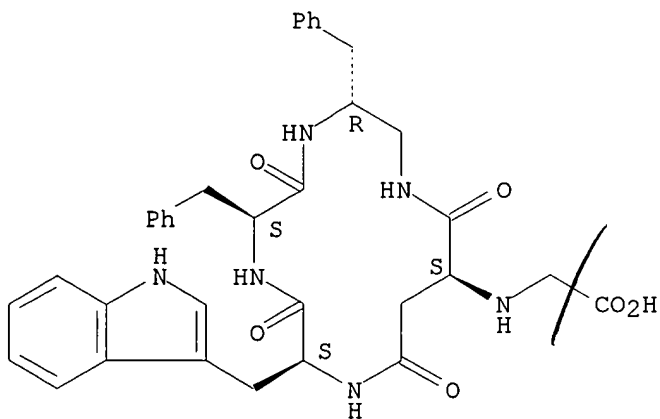


RN 211689-52-0 CAPLUS  
 CN L-Phenylalanine, N-[(2R)-2-amino-3-phenylpropyl]-N2-(carboxymethyl)-L-  
 .alpha.-asparaginyl-L-tryptophyl-, (3.fwdarw.1)-lactam,  
 mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

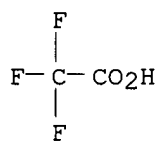
CRN 211689-51-9  
 CMF C35 H38 N6 O6

Absolute stereochemistry.



CM 2

CRN 76-05-1  
 CMF C2 H F3 O2



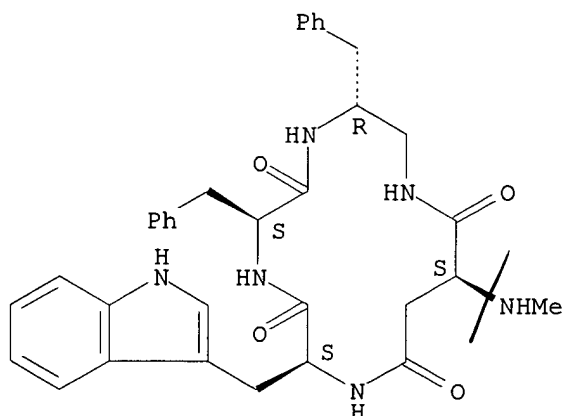
IT 211689-29-1P 211689-38-2P 211689-40-6P  
 211689-42-8P 211689-46-2P 211689-48-4P  
 211689-50-8P 211689-54-2P 211689-55-3P  
 211689-57-5P 211689-59-7P

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (monocyclic compds. with four bifunctional residues having NK-2 antagonist action)

RN 211689-29-1 CAPLUS

CN L-Phenylalanine, N-[(2R)-2-amino-3-phenylpropyl]-N2-methyl-L-.alpha.-asparaginyl-L-tryptophyl-, (3.fwdarw.1)-lactam (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 211689-38-2 CAPLUS

CN L-Phenylalanine, N-[(2R)-2-amino-3-phenylpropyl]-N2-(1H-tetrazol-5-ylmethyl)-L-.alpha.-asparaginyl-L-tryptophyl-, (3.fwdarw.1)-lactam, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

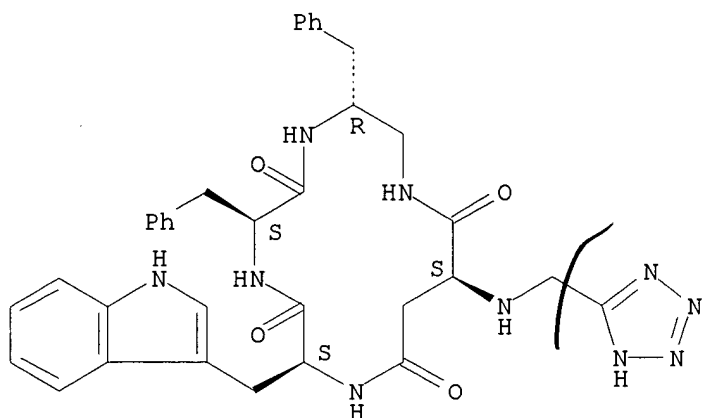
CM 1

CRN 211689-37-1

CMF C35 H38 N10 O4

Absolute stereochemistry.

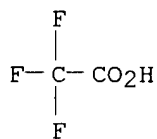
09/762,522



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 211689-40-6 CAPLUS

CN Cyclo[(3S)-4-[[[(2R)-2-amino-3-phenylpropyl]amino]-3-(4-morpholinyl)-4-oxobutanoyl-L-tryptophyl-L-phenylalanyl], mono(trifluoroacetate) (9CI)  
(CA INDEX NAME)

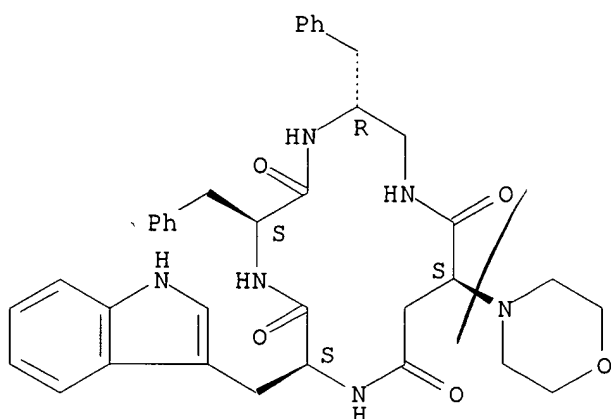
CM 1

CRN 211689-39-3

CMF C37 H42 N6 O5

Absolute stereochemistry.

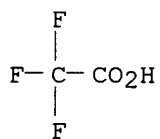
09/762,522



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 211689-42-8 CAPLUS

CN L-Phenylalanine, N-[(2R)-2-amino-3-phenylpropyl]-N<sub>2</sub>,N<sub>2</sub>-dimethyl-L-.alpha.-asparaginy-L-tryptophyl-, (3.fwdarw.1)-lactam, mono(trifluoroacetate)  
(9CI) (CA INDEX NAME)

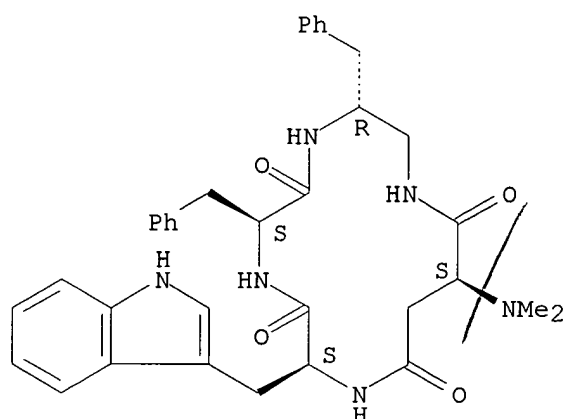
CM 1

CRN 211689-41-7

CMF C35 H40 N6 O4

Absolute stereochemistry.

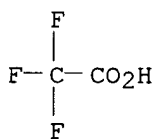
09/762,522



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 211689-46-2 CAPLUS

CN L-Phenylalanine, N-[(2R)-2-amino-3-phenylpropyl]-N2,N2-bis(2-hydroxyethyl)-L-.alpha.-asparaginyl-L-tryptophyl-, (3.fwdarw.1)-lactam, mono(trifluoroacetate) (salt) (9CI) (CA INDEX NAME)

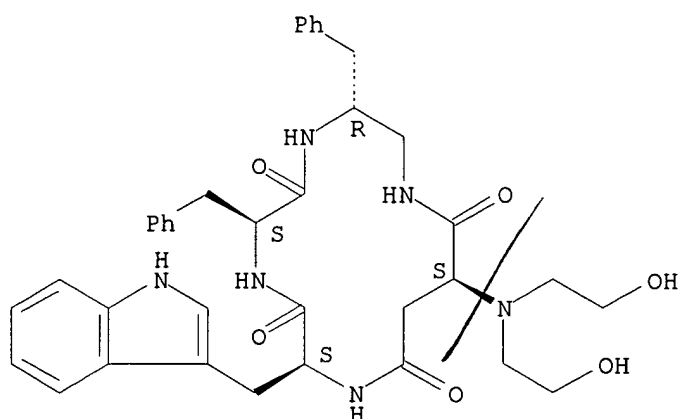
CM 1

CRN 211689-45-1

CMF C37 H44 N6 O6

Absolute stereochemistry.

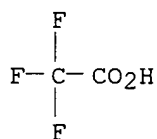
09/762,522



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 211689-48-4 CAPLUS

CN L-Phenylalanine, N-[(2R)-2-amino-3-phenylpropyl]-N2-[(2R)-2,3-dihydroxypropyl]-L-.alpha.-asparaginy-L-tryptophyl-, (3.fwdarw.1)-lactam, mono(trifluoroacetate) (salt) (9CI) (CA INDEX NAME)

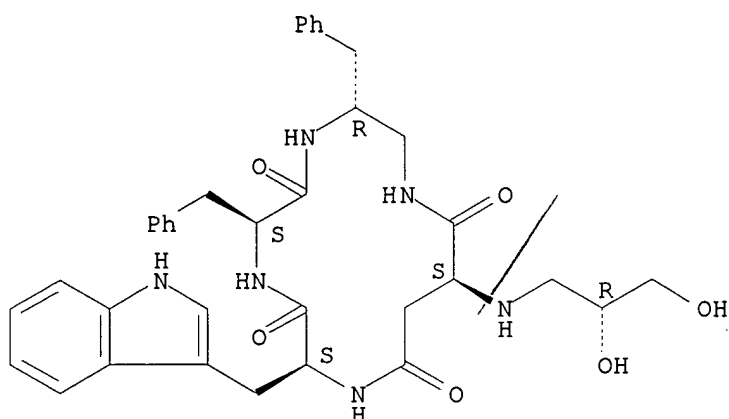
CM 1

CRN 211689-47-3

CMF C36 H42 N6 O6

Absolute stereochemistry.

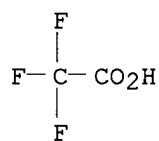
09/762,522



CM 2

CRN 76-05-1

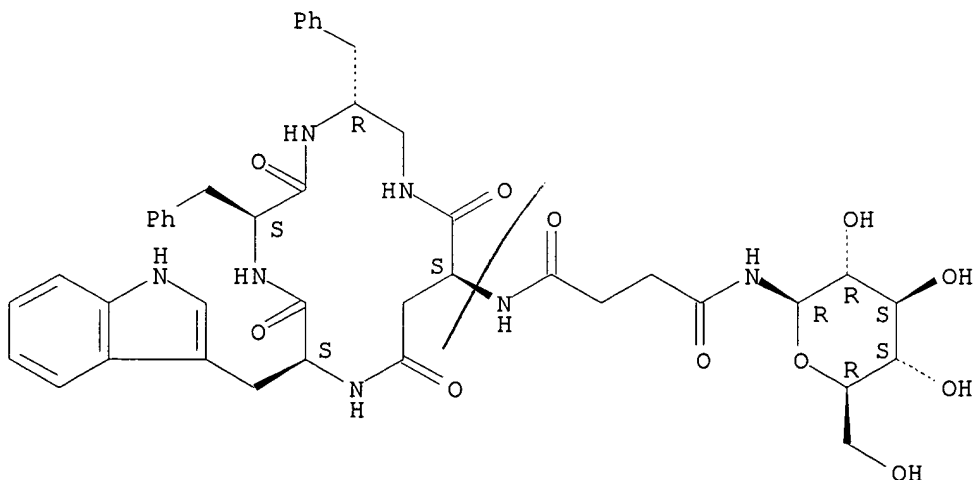
CMF C2 H F3 O2



RN 211689-50-8 CAPLUS

CN L-Phenylalanine, N-[(2R)-2-amino-3-phenylpropyl]-N2-[4-(.beta.-D-glucopyranosylamino)-1,4-dioxobutyl]-L-.alpha.-asparaginyl-L-tryptophyl-, (3.fwdarw.1)-lactam (9CI) (CA INDEX NAME)

Absolute stereochemistry.



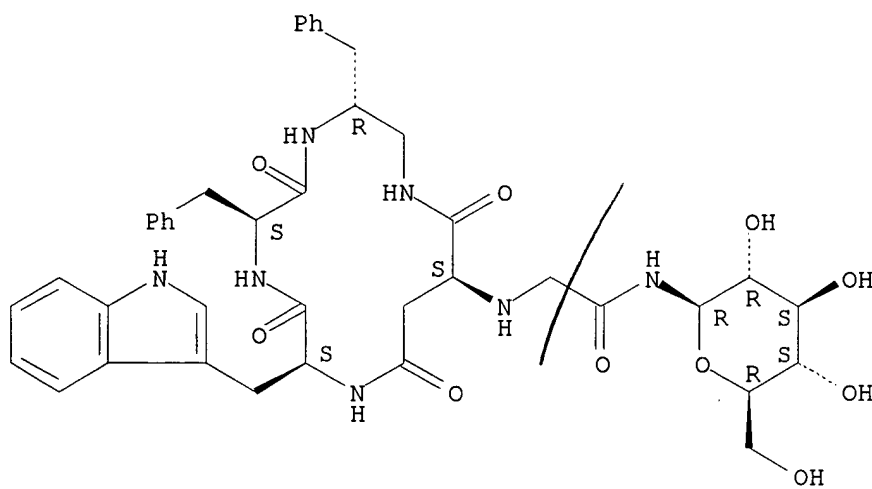
09/762,522

RN 211689-54-2 CAPLUS  
CN L-Phenylalanine, N-[(2R)-2-amino-3-phenylpropyl]-N2-[2-(.beta.-D-glucopyranosylamino)-2-oxoethyl]-L-.alpha.-asparaginy-L-tryptophyl-, (3.fwdarw.1)-lactam, mono(trifluoroacetate) (salt) (9CI) (CA INDEX NAME)

CM 1

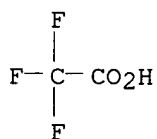
CRN 211689-53-1  
CMF C41 H49 N7 O10

Absolute stereochemistry.



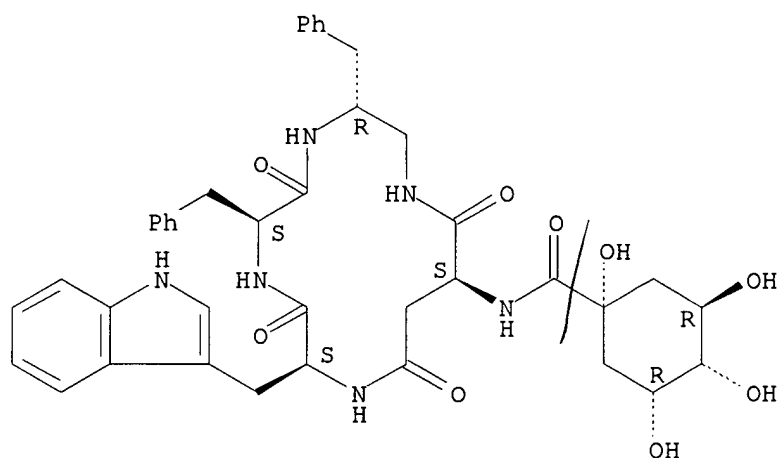
CM 2

CRN 76-05-1  
CMF C2 H F3 O2



RN 211689-55-3 CAPLUS  
CN L-Phenylalanine, N-[(2R)-2-amino-3-phenylpropyl]-N2-[[ (1.alpha.,3R,4.alpha.,5R)-1,3,4,5-tetrahydroxycyclohexyl]carbonyl]-L-.alpha.-asparaginy-L-tryptophyl-, (3.fwdarw.1)-lactam (9CI) (CA INDEX NAME)

Absolute stereochemistry.

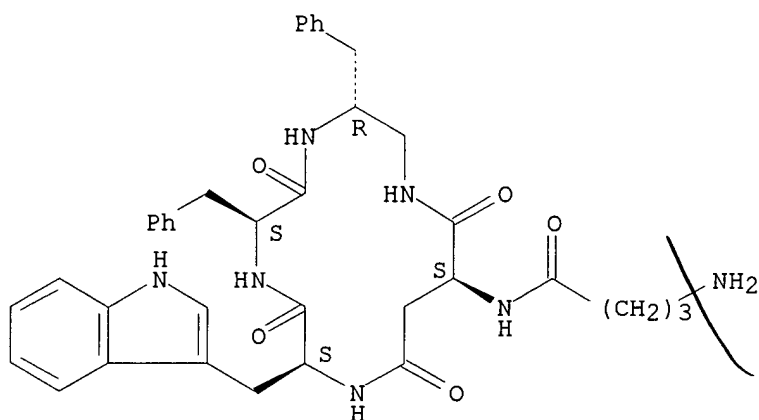


RN 211689-57-5 CAPLUS  
 CN L-Phenylalanine, N2-(4-amino-1-oxobutyl)-N-[(2R)-2-amino-3-phenylpropyl]-L-  
 .alpha.-asparaginyl-L-tryptophyl-, (3.fwdarw.1)-lactam,  
 mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 211689-56-4  
 CMF C37 H43 N7 O5

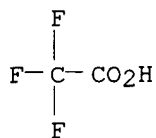
Absolute stereochemistry.



CM 2

CRN 76-05-1  
 CMF C2 H F3 O2

09/762,522

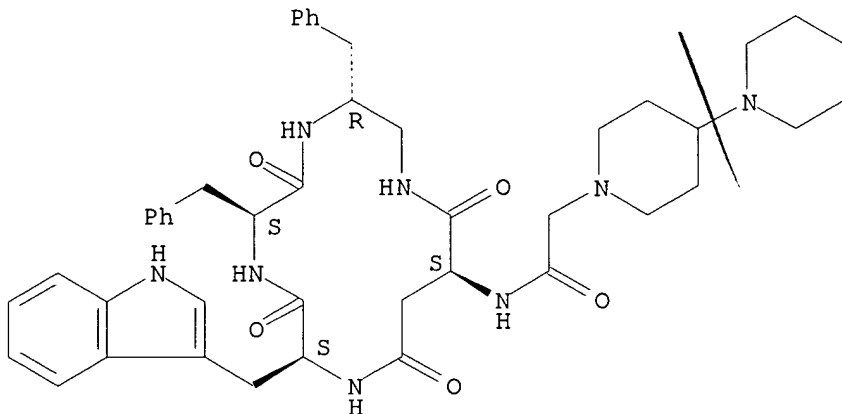


RN 211689-59-7 CAPLUS  
CN L-Phenylalanine, N-[(2R)-2-amino-3-phenylpropyl]-N2-([1,4'-bipiperidin]-1'-ylacetyl)-L-.alpha.-asparaginy-L-tryptophyl-, (3.fwdarw.1)-lactam, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

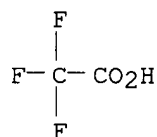
CRN 211689-58-6  
CMF C45 H56 N8 O5

Absolute stereochemistry.



CM 2

CRN 76-05-1  
CMF C2 H F3 O2

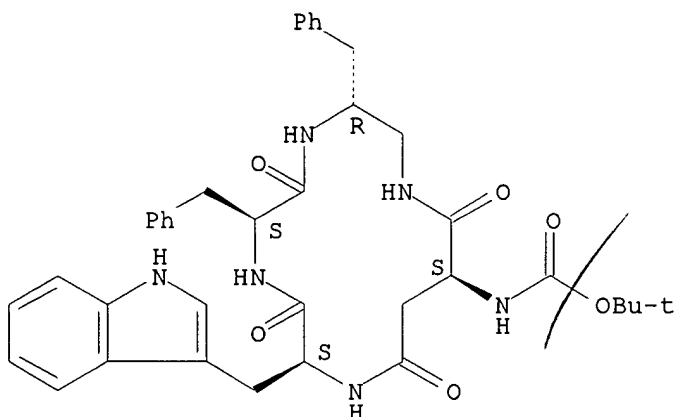


IT **211689-74-6P 211689-80-4P 211689-81-5P**  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)  
(monocyclic compds. with four bifunctional residues having NK-2 antagonist action)  
RN 211689-74-6 CAPLUS  
CN L-Phenylalanine, N-[(2R)-2-amino-3-phenylpropyl]-N2-[(1,1-dimethylethoxy)carbonyl]-L-.alpha.-asparaginy-L-tryptophyl-,

09/762,522

(3.fwdarw.1)-lactam (9CI) (CA INDEX NAME)

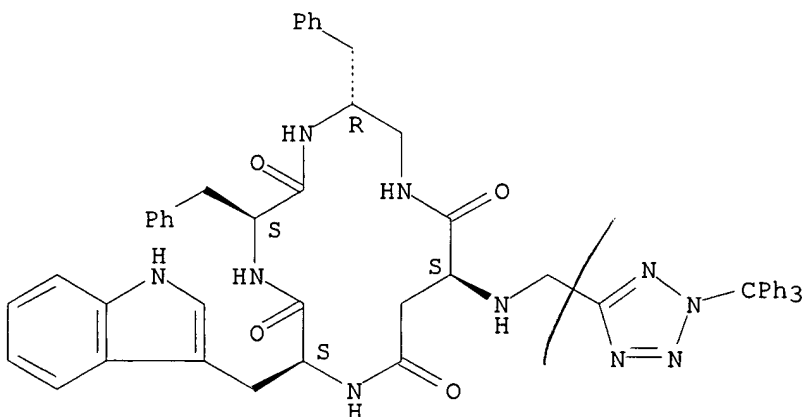
Absolute stereochemistry.



RN 211689-80-4 CAPLUS

CN L-Phenylalanine, N-[(2R)-2-amino-3-phenylpropyl]-N2-[[2-(triphenylmethyl)-2H-tetrazol-5-yl]methyl]-L-.alpha.-asparaginyL-L-tryptophyl-, (3.fwdarw.1)-lactam (9CI) (CA INDEX NAME)

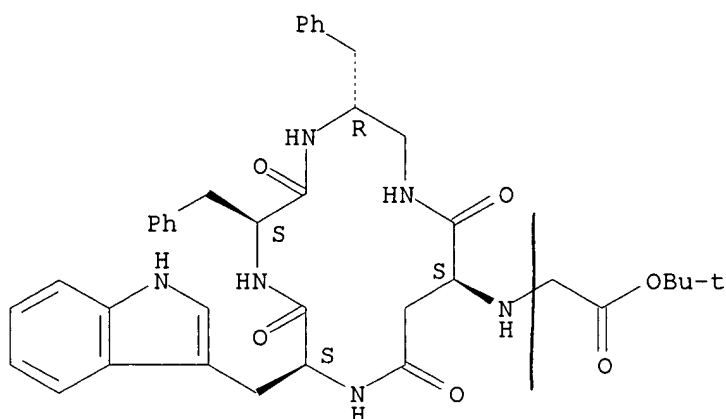
Absolute stereochemistry.



RN 211689-81-5 CAPLUS

CN L-Phenylalanine, N-[(2R)-2-amino-3-phenylpropyl]-N2-[2-(1,1-dimethylethoxy)-2-oxoethyl]-L-.alpha.-asparaginy-L-tryptophyl-, (3.fwdarw.1)-lactam (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 211689-75-7P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(monocyclic compds. with four bifunctional residues having NK-2  
antagonist action)

RN 211689-75-7 CAPLUS

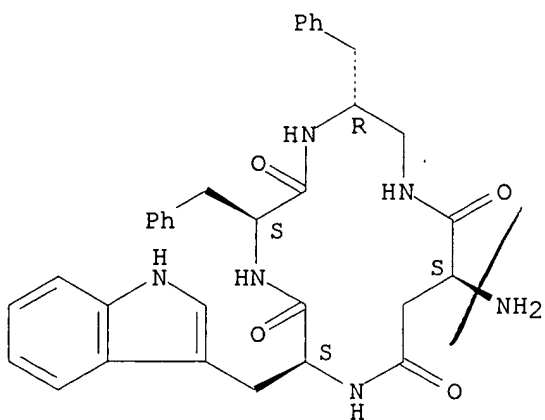
CN L-Phenylalanine, N-[(2R)-2-amino-3-phenylpropyl]-L-.alpha.-asparaginyl-L-tryptophyl-, (3.fwdarw.1)-lactam, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 211689-25-7

CMF C33 H36 N6 O4

Absolute stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2

09/762,522

